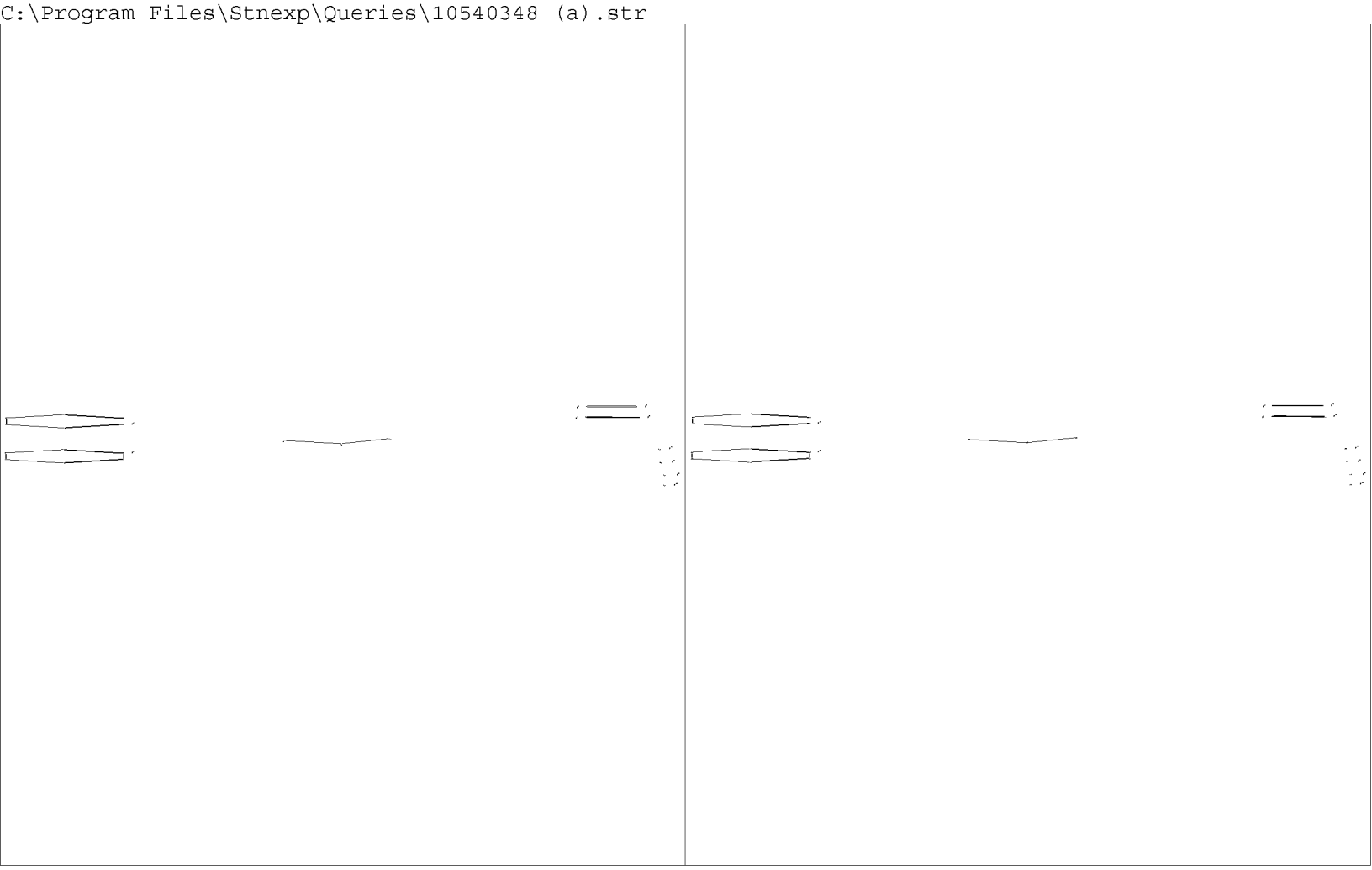
C:\Program Files\Stnexp\Queries\10540348 (a).str



chain nodes :
    8 9 10 11 25 27 28 29 30 31 39
ring nodes :
    1 2 3 4 5 6 16 17 18 19 20 21
chain bonds :
    8-9 10-11 25-27 27-28
ring bonds :
    1-2 1-6 2-3 3-4 4-5 5-6 16-17 16-21 17-18 18-19 19-20 20-21
exact/norm bonds :
    25-27 27-28
exact bonds :
    8-9 10-11
normalized bonds :
    1-2 1-6 2-3 3-4 4-5 5-6 16-17 16-21 17-18 18-19 19-20 20-21
isolated ring systems :
    containing 1 : 16 :

G1:[*1],[*2]

G2:[*3-*4],[*5-*6]

G3:[*7],[*8],[*9],[*10]

Match level :
    1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 10:CLASS 11:CLASS 16:Atom
    17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 25:CLASS 27:CLASS 28:CLASS 29:Atom 30:Atom
    31:Atom 39:Atom
Generic attributes :
    29:
    Saturation   : Unsaturated
    Number of Hetero Atoms : 2 or more
    Type of Ring System   : Polycyclic
    30:
    Saturation   : Unsaturated

```
    Number of Carbon Atoms : less than 7
    Number of Hetero Atoms : 2 or more
    Type of Ring System    : Monocyclic
    31:
    Saturation             : Unsaturated
    Number of Carbon Atoms : less than 7
    Number of Hetero Atoms : 2 or more
    Type of Ring System    : Monocyclic
    39:
    Saturation             : Unsaturated
    Number of Carbon Atoms : less than 7
    Number of Hetero Atoms : 2 or more
    Type of Ring System    : Monocyclic

Element Count :
    Node 29: Limited
        C,C3
        N,N2

    Node 30: Limited
        C,C3
        N,N1
        O,O1
        S,S0

    Node 31: Limited
        C,C3
        N,N1
        S,S1
        O,O0

    Node 39: Limited
        C,C3
        N,N2
        O,O0
        S,S0
```

=>
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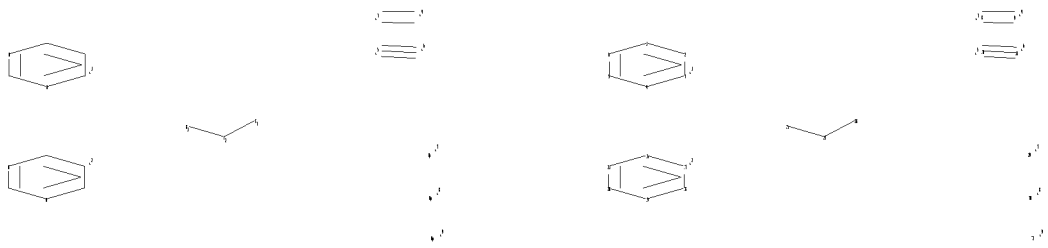

chain nodes :
8 9 10 11 25 27 28 29 30 32
ring nodes :
1 2 3 4 5 6 16 17 18 19 20 21
chain bonds :
8-9 10-11 25-27 27-28
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 16-17 16-21 17-18 18-19 19-20 20-21
exact/norm bonds :

```
25-27  27-28
exact bonds :
8-9  10-11
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6  16-17  16-21  17-18  18-19  19-20  20-21
isolated ring systems :
containing 1 : 16 :


G1:[*1],[*2]

G2:[*3-*4],[*5-*6]

G3:[*7],[*8],[*9]

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  8:CLASS  9:CLASS  10:CLASS
11:CLASS  16:Atom  17:Atom  18:Atom  19:Atom  20:Atom  21:Atom  25:CLASS  27:CLASS
28:CLASS  29:Atom  30:Atom  32:Atom
Generic attributes :
29:
Saturation             : Unsaturated
Number of Hetero Atoms : 2 or more
30:
Saturation             : Unsaturated
Number of Carbon Atoms : less than 7
Number of Hetero Atoms : 2 or more
Type of Ring System    : Monocyclic
32:
Saturation             : Unsaturated
Number of Carbon Atoms : less than 7
Number of Hetero Atoms : 2 or more
Type of Ring System    : Monocyclic

Element Count :
Node 29: Limited
    C,C3
    N,N2

Node 30: Limited
    C,C3
    N,N1
    O,O1
    S,S0

Node 32: Limited
    C,C3
    N,N1
    S,S1
    O,O0




L1      STRUCTURE UPLOADED
```

```
=> d l1
L1 HAS NO ANSWERS
L1              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.


=> s l1 sss sam
SAMPLE SEARCH INITIATED 23:09:56 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -     4500 TO ITERATE

 44.4% PROCESSED     2000 ITERATIONS                                 8 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:        85977 TO    94023
PROJECTED ANSWERS:             106 TO      614

L2            8 SEA SSS SAM L1

=> =>
Uploading C:\Program Files\Stnexp\Queries\10540348 (a).str
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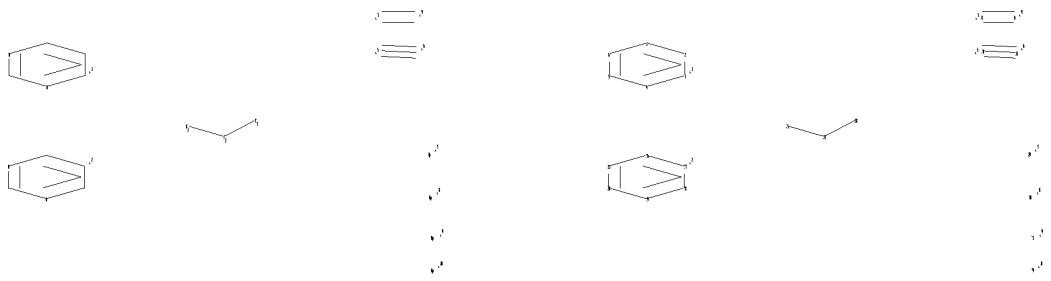

chain nodes :
8 9 10 11 25 27 28 29 30 31 39
ring nodes :
1 2 3 4 5 6 16 17 18 19 20 21
chain bonds :
8-9 10-11 25-27 27-28
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 16-17 16-21 17-18 18-19 19-20 20-21

```
exact/norm bonds :
25-27  27-28
exact bonds :
8-9  10-11
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6  16-17  16-21  17-18  18-19  19-20  20-21
isolated ring systems :
containing 1 : 16 :


G1:[*1],[*2]

G2:[*3-*4],[*5-*6]

G3:[*7],[*8],[*9],[*10]

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  8:CLASS  9:CLASS  10:CLASS
11:CLASS  16:Atom  17:Atom  18:Atom  19:Atom  20:Atom  21:Atom  25:CLASS  27:CLASS
28:CLASS  29:Atom  30:Atom  31:Atom  39:Atom
Generic attributes :
29:
Saturation             : Unsaturated
Number of Hetero Atoms : 2 or more
Type of Ring System    : Polycyclic
30:
Saturation             : Unsaturated
Number of Carbon Atoms : less than 7
Number of Hetero Atoms : 2 or more
Type of Ring System    : Monocyclic
31:
Saturation             : Unsaturated
Number of Carbon Atoms : less than 7
Number of Hetero Atoms : 2 or more
Type of Ring System    : Monocyclic
39:
Saturation             : Unsaturated
Number of Carbon Atoms : less than 7
Number of Hetero Atoms : 2 or more
Type of Ring System    : Monocyclic

Element Count :
Node 29: Limited
    C,C3
    N,N2

Node 30: Limited
    C,C3
    N,N1
    O,O1
    S,S0

Node 31: Limited
    C,C3
    N,N1
    S,S1
    O,O0
```

```
Node 39: Limited
    C,C3
    N,N2
    O,O0
    S,S0




L3      STRUCTURE UPLOADED

=> d l3
L3 HAS NO ANSWERS
L3              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.


=> s l3 sss sam
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SAMPLE SCREEN SEARCH COMPLETED -     4500 TO ITERATE

 44.4% PROCESSED     2000 ITERATIONS                                5 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:         85977 TO    94023
PROJECTED ANSWERS:               24 TO      426

L4            5 SEA SSS SAM L3

=> =>
Uploading C:\Program Files\Stnexp\Queries\10540348 (b).str
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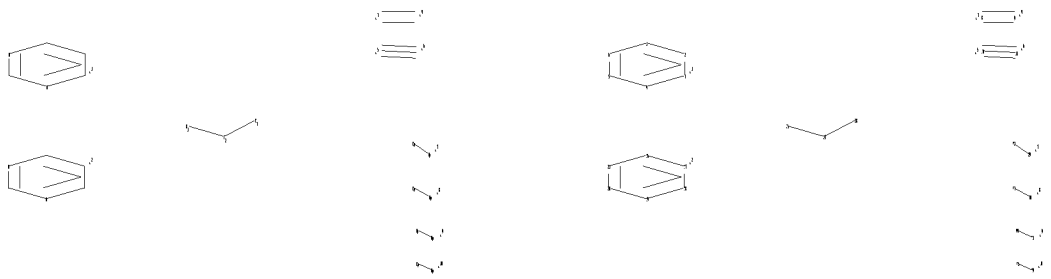


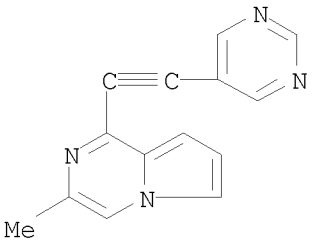
chain nodes :
8 9 10 11 25 27 28 29 30 31 39 42 43 44 45
ring nodes :
1 2 3 4 5 6 16 17 18 19 20 21
chain bonds :
8-9 10-11 25-27 27-28 29-42 30-43 31-44 39-45
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 16-17 16-21 17-18 18-19 19-20 20-21

```
exact/norm bonds :
25-27  27-28  29-42  30-43  31-44  39-45
exact bonds :
8-9  10-11
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6  16-17  16-21  17-18  18-19  19-20  20-21
isolated ring systems :
containing 1 : 16 :


G1:[*1],[*2]

G2:[*3-*4],[*5-*6]

G3:[*7],[*8],[*9],[*10]

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  8:CLASS  9:CLASS  10:CLASS
11:CLASS  16:Atom  17:Atom  18:Atom  19:Atom  20:Atom  21:Atom  25:CLASS  27:CLASS
28:CLASS  29:Atom  30:Atom  31:Atom  39:Atom  42:Atom  43:Atom  44:Atom  45:Atom
Generic attributes :
29:
Saturation             : Unsaturated
Number of Hetero Atoms : 2 or more
Type of Ring System    : Polycyclic
30:
Saturation             : Unsaturated
Number of Carbon Atoms : less than 7
Number of Hetero Atoms : 2 or more
Type of Ring System    : Monocyclic
31:
Saturation             : Unsaturated
Number of Carbon Atoms : less than 7
Number of Hetero Atoms : 2 or more
Type of Ring System    : Monocyclic
39:
Saturation             : Unsaturated
Number of Carbon Atoms : less than 7
Number of Hetero Atoms : 2 or more
Type of Ring System    : Monocyclic
42:
Saturation             : Unsaturated
43:
Saturation             : Unsaturated
44:
Saturation             : Unsaturated
45:
Saturation             : Unsaturated

Element Count :
Node 29: Limited
    C,C3
    N,N2

Node 30: Limited
    C,C3
    N,N1
```

```
    O,O1
    S,S0

Node 31: Limited
    C,C3
    N,N1
    S,S1
    O,O0

Node 39: Limited
    C,C3
    N,N2
    O,O0
    S,S0




L5      STRUCTURE UPLOADED

=> d l5
L5 HAS NO ANSWERS
L5              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.


=> s l5 sss sam
SAMPLE SEARCH INITIATED 23:16:24 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -     4500 TO ITERATE

 44.4% PROCESSED     2000 ITERATIONS                                0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:        85977 TO    94023
PROJECTED ANSWERS:               0 TO        0

L6            0 SEA SSS SAM L5

=> s l3 sss ful
FULL SEARCH INITIATED 23:18:17 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    89937 TO ITERATE

100.0% PROCESSED    89937 ITERATIONS                             275 ANSWERS
SEARCH TIME: 00.00.01

L7          275 SEA SSS FUL L3

=> => s l7
L8          86 L7
```

=> d l8 1-86 bib,ab,hitstr

L8 ANSWER 1 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2008:338438 CAPLUS
DN 148:528844
TI Phenylethynyl-pyrrolo[1,2-a]pyrazine: A new potent and selective tool in the mGluR5 antagonists arena
AU Micheli, Fabrizio; Bertani, Barbara; Bozzoli, Andrea; Crippa, Luca; Cavanni, Paolo; Di Fabio, Romano; Donati, Daniele; Marzorati, Paola; Merlo, Giancarlo; Paio, Alfredo; Perugini, Lorenzo; Zarantonello, Paola
CS Psychiatry Centre of Excellence for Drug Discovery, GlaxoSmithKline, Verona, 37135, Italy
SO Bioorganic & Medicinal Chemistry Letters (2008), 18(6), 1804-1809
CODEN: BMCLE8; ISSN: 0960-894X
PB Elsevier Ltd.
DT Journal
LA English
AB The synthesis and the structure activity of a new series of pyrrolo[1,2-a]pyrazine is reported. These mols. are potent and selective noncompetitive mGluR5 antagonists and may shed new light on the pattern of substitution tolerated by this receptor.
IT 1025052-65-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(phenylethynyl-pyrrolo[1,2-a]pyrazine as new potent and selective tool in mGluR5 antagonists arena)
RN 1025052-65-6 CAPLUS
CN Pyrrolo[1,2-a]pyrazine, 3-methyl-1-[2-(5-pyrimidinyl)ethynyl]- (CA INDEX NAME)



RE.CNT 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 2 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2007:1450137 CAPLUS
DN 148:62071
TI Anti-infection augmentation foamable compositions and kit and uses thereof
IN Tamarkin, Dov; Friedman, Doron; Eini, Meir
PA Foamix Ltd., Israel
SO U.S. Pat. Appl. Publ., 43pp., Cont.-in-part of U.S. Ser. No. 448,490.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 26

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 20070292355	A1	20071220	US 2007-732547	20070404
	WO 2004037225	A2	20040506	WO 2003-IB5527	20031024
	WO 2004037225	A3	20041229		
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	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	US 20050031547	A1	20050210	US 2004-835505	20040428
	US 20050069566	A1	20050331	US 2004-911367	20040804
	US 20050074414	A1	20050407	US 2004-922358	20040820
	AU 2004313285	A1	20050929	AU 2004-313285	20041216
	US 20050186142	A1	20050825	US 2005-41921	20050124
	ZA 2005003298	A	20060830	ZA 2005-3298	20050425
	US 20060140984	A1	20060629	US 2005-532618	20051222
	AU 2006201878	A1	20070927	AU 2006-201878	20060504
	US 20060269485	A1	20061130	US 2006-448490	20060607
	AU 2006339311	A2	20070907	AU 2006-339311	20060607
	AU 2006339311	A1	20070907		
	CA 2611577	A1	20070907	CA 2006-2611577	20060607
	WO 2007099396	A2	20070907	WO 2006-IB3975	20060607
	WO 2007099396	A3	20080313		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW				
	RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA				
	EP 1919449	A2	20080514	EP 2006-847249	20060607
	R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, MK, RS				
	US 20070280891	A1	20071206	US 2006-645444	20061226

	US 20080050317	A1	20080228	US 2007-894668	20070820
PRAI	IL 2002-152486	A	20021025		
	US 2002-429546P	P	20021129		
	US 2003-492385P	P	20030804		
	US 2003-497648P	P	20030825		
	WO 2003-IB5527	W	20031024		
	US 2003-530015P	P	20031216		
	US 2004-835505	A2	20040428		
	US 2004-911367	A2	20040804		
	US 2004-922358	A2	20040820		
	US 2005-41921	A2	20050124		
	US 2005-688244P	P	20050607		
	US 2005-532618	A2	20051222		
	US 2006-789186P	P	20060404		
	US 2006-448490	A2	20060607		
	US 2006-861620P	P	20061129		
	US 2007-880434P	P	20070112		
	WO 2006-IB3975	W	20060607		

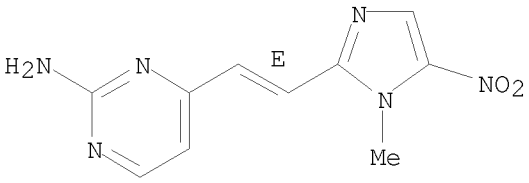
AB This invention relates to anti-infective foamable composition and kits include a foamable carrier; a therapeutically safe and effective concentration of an anti-infective agent; an augmenting agent selected from the group consisting of a keratolytic agent and a skin penetration enhancer; and a propellant. The composition is housed in a container and upon release is expandable to form a breakable foam. The foamable carrier is selected to generate a foam of good or excellent quality in the presence of the augmenting agent and anti-infective agent. Methods for treating, alleviating or preventing a disorder of the skin, a body cavity or mucosal surface, wherein the disorder involves a fungal, bacterial or viral infection as one of its etiol. factors, is described. Thus, foamable composition was prepared containing PEG 400 91.65%, hydroxypropyl cellulose 0.475, steareth 2 1.88%, salicylic acid 5.0%, and ciclopiroxolamine 1.0%.

IT 62973-76-6, Azanidazole
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(anti-infection augmentation foamable compns. and kit and uses thereof)

RN 62973-76-6 CAPLUS

CN 2-Pyrimidinamine, 4-[(1E)-2-(1-methyl-5-nitro-1H-imidazol-2-yl)ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.



L8 ANSWER 3 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2007:1146854 CAPLUS
DN 147:398630
TI Kit for treating skin infection
IN Shemer, Avner
PA Israel
SO PCT Int. Appl., 28pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2007113830	A2	20071011	WO 2007-IL437	20070410

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

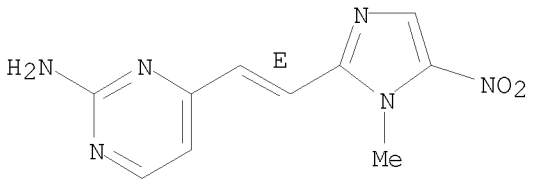
PRAI US 2006-219484 A 20060404

AB The invention provides a therapeutic composition, simultaneously containing (1) at least one polar solvent, selected from the group of a short-chain mono-alc. and a diol; (2) between about 2% and about 25% of at least two keratolytic agents; and (3) a therapeutically safe and effective concentration of a antifungal agent. It further provides a kit, consisting of an occlusive device and a therapeutic composition, useful for treatment of fungal skin infection.

IT 62973-76-6, Azanidazole
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(kit for treating skin infection)

RN 62973-76-6 CAPLUS
CN 2-Pyrimidinamine, 4-[(1E)-2-(1-methyl-5-nitro-1H-imidazol-2-yl)ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.

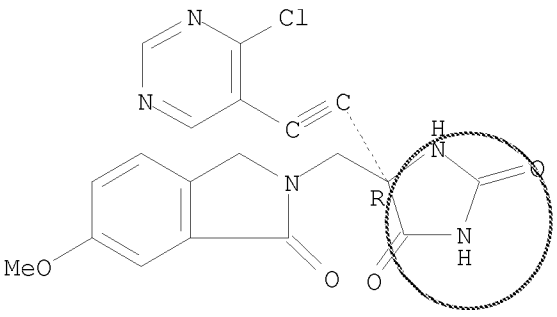


L8 ANSWER 4 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2007:1061197 CAPLUS
DN 147:385984
TI Imidazolidinedione derivatives and their preparation, pharmaceutical compositions, and use for the treatment of inflammatory disorders
IN Yu, Wensheng; Tong, Ling; Chen, Lei; Kozlowski, Joseph A.; Lavey, Brian J.; Shih, Neng-Yang; Madison, Vincent S.; Zhou, Guowei; Orth, Peter; Guo, Zhuyan; Wong, Michael K. C.; Yang, De-Yi; Kim, Seong Heon; Shankar, Bandarpalle B.; Siddiqui, M. Arshad; Rosner, Kristin E.; Dai, Chaoyang; Popovici-Muller, Janeta; Girijavallabhan, Vinay M.; Li, Dansu; Rizvi, Razia; Micula, Aneta M.; Feltz, Robert
PA Schering Corporation, USA
SO U.S. Pat. Appl. Publ., 430pp., Cont.-in-part of U.S. Ser. No. 333,663. CODEN: USXXCO
DT Patent
LA English
FAN.CNT 3

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 20070219218	A1	20070920	US 2007-653676	20070116
	US 20060205797	A1	20060914	US 2005-180863	20050713
	US 20060276506	A1	20061207	US 2006-333663	20060117
PRAI	US 2004-588502P	P	20040716		
	US 2005-180863	A2	20050713		
	US 2006-333663	A2	20060117		

OS MARPAT 147:385984
AB This invention relates to imidazolidinedione derivs. I [X = S, (un)substituted CH2 or NH; T = H, alkyl, aryl, etc.; U = absent, a bond, O, etc.; V = absent, alkyl, aryl, etc.; Y, Z = absent, a bond, O, etc.; R1, R2 = H, halo, alkyl, etc.; R4 = H, alkyl, cycloalkyl, etc.] or a pharmaceutically acceptable salt, solvate, ester or isomer thereof, which can be useful for the treatment of diseases or conditions mediated by MMPs, ADAMs, TACE, aggrecanase, TNF- or combinations thereof. Thus, amidation of 5-methoxy-2-nitrobenzoic acid with 5-(aminomethyl)-5-methylimidazolidine-2,4-dione followed by reduction and cyclization of the resulting N-(2,4-dioxo-5-methylimidazolidin-5-ylmethyl) 5-methoxy-2-nitrobenzamide afforded the title compound II. The invention compds. I were evaluated for their antiinflammatory activity. For example, II exhibited Ki value in the range of 100 to 1000 nM.
IT 950176-39-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of substituted imidazolidinediones for treatment and prevention of inflammatory disorders)
RN 950176-39-3 CAPLUS
CN 2,4-Imidazolidinedione, 5-[2-(4-chloro-5-pyrimidinyl)ethynyl]-5-[(1,3-dihydro-6-methoxy-1-oxo-2H-isoindol-2-yl)methyl]-, (5R)- (CA INDEX NAME)

Absolute stereochemistry.

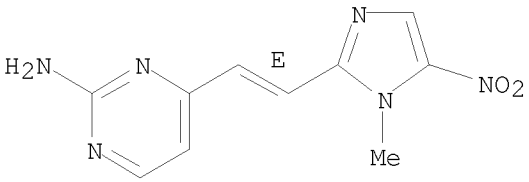

N
Cl
N
C
C
N
R
H
N
O
N
H
MeO
O
O

L8 ANSWER 5 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2007:1016569 CAPLUS
DN 148:503081
TI Novel drug delivery system
IN Nadkarni, Sunil Sadanand; Vaya, Navin; Karan, Rajesh Singh; Gupta, Vinod Kumar
PA Torrent Pharmaceuticals Limited, India
SO Indian Pat. Appl., 80pp., Addn. of Indian Appl. No. 2004MU198.
CODEN: INXXBQ
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI IN 2005MU01012	A	20070831	IN 2005-MU1012	20050826
PRAI IN 2004-MU198	A0	20040220		

AB A novel modified release dosage form comprising of a high solubility active ingredient, which utilizes dual retard technique to effectively reduce the quantity of release controlling agents. Present invention can optionally comprise addnl. another active ingredient as an immediate release form or modified release form. Present invention also relates to a process for preparing the said formulation.
IT 62973-76-6, Azanidazole
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(novel drug delivery system)
RN 62973-76-6 CAPLUS
CN 2-Pyrimidinamine, 4-[(1E)-2-(1-methyl-5-nitro-1H-imidazol-2-yl)ethenyl]-
(CA INDEX NAME)

Double bond geometry as shown.



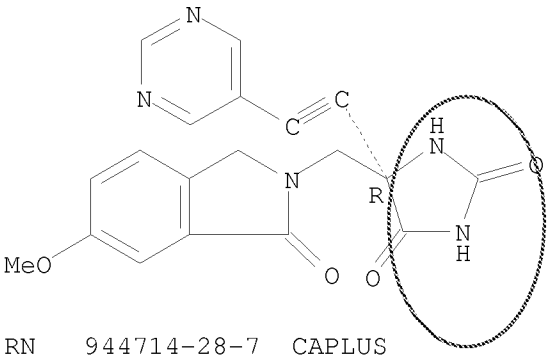
L8 ANSWER 6 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2007:814060 CAPLUS
DN 147:211876
TI Hydantoin derivatives for the treatment of inflammatory disorders and their preparation
IN Lavey, Brian J.; Kozlowski, Joseph A.; Zhou, Guowei; Tong, Ling; Yu, Wensheng; Wong, Michael K. C.; Shankar, Bandarpalle B.; Shih, Neng-Yang; Siddiqui, M. Arshad; Rosner, Kristin E.; Dai, Chaoyang; Popovici-Muller, Janeta; Girijavallabhan, Vinay M.; Li, Dansu; Rizvi, Razia; Chen, Lei; Yang, De-Yi; Feltz, Robert; Kim, Seong-Heon
PA Schering Corporation, USA
SO PCT Int. Appl., 294pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2007084451	A1	20070726	WO 2007-US1025	20070116
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW				
	RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	US 20070197564	A1	20070823	US 2007-653511	20070116
	US 20070265299	A1	20071115	US 2007-653798	20070116
PRAI	US 2006-759300P	P	20060117		

OS MARPAT 147:211876
AB This invention relates to compds. of the formula: I; or a pharmaceutically acceptable salt, solvate or isomer thereof, which can be useful for the treatment of diseases or conditions mediated by MMPs, ADAMs, TACE, aggrecanase, TNF-α or combinations thereof. Compds. of formula I wherein ring A is (hetero)aryl; X is S, O, SO2, S, (un)substituted C1-3 alkyl, and NR3; T is alkynyl; V is H, alkyl, cycloalkyl, cycloalkenyl, (hetero)aryl, etc.; Y and Z are independently (un)substituted C1-3 alkyl, NH and derivs, CONH and derivs., NHCO and derivs., NHCONH and derivs., SO2Nh and derivs., etc.; R1, R2, and R3 are independently H, CN, alkynyl, halo, (halo)alkyl, cycloalkyl, (hetero)aryl, etc.; and their pharmaceutically acceptable salts, solvates, esters and isomers thereof, are claimed. Example compound II was prepared by a general procedure (procedure given). All the invention compds. were evaluated for their antiinflammatory activity. From the assay, it was determined that compound II exhibited Ki value in the range from 5 to less than 25 nM.
IT 944714-25-4P 944714-28-7P 944717-14-0P
944717-15-1P 944717-41-3P 944717-89-9P
944717-95-7P 944718-00-7P 944718-01-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of hydantoin derivs. for treatment of inflammatory disorders

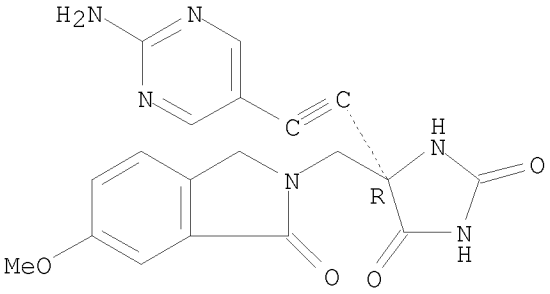
and other diseases)
RN 944714-25-4 CAPLUS
CN 2,4-Imidazolidinedione, 5-[(1,3-dihydro-6-methoxy-1-oxo-2H-isoindol-2-yl)methyl]-5-[2-(5-pyrimidinyl)ethynyl]-, (5R)- (CA INDEX NAME)

Absolute stereochemistry.



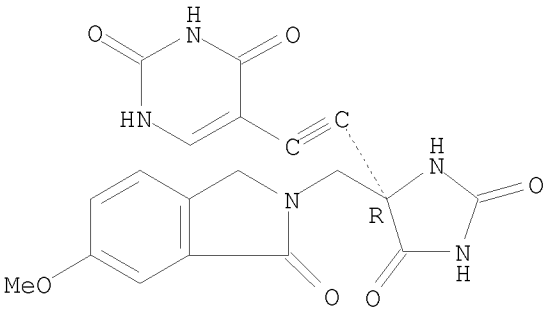
RN 944714-28-7 CAPLUS
CN 2,4-Imidazolidinedione, 5-[2-(2-amino-5-pyrimidinyl)ethynyl]-5-[(1,3-dihydro-6-methoxy-1-oxo-2H-isoindol-2-yl)methyl]-, (5R)- (CA INDEX NAME)

Absolute stereochemistry.



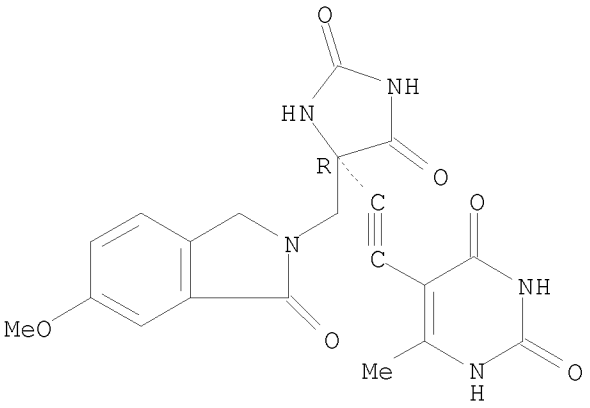
RN 944717-14-0 CAPLUS
CN 2,4(1H,3H)-Pyrimidinedione, 5-[2-[(4R)-4-[(1,3-dihydro-6-methoxy-1-oxo-2H-isoindol-2-yl)methyl]-2,5-dioxo-4-imidazolidinyl]ethynyl]- (CA INDEX NAME)

Absolute stereochemistry.



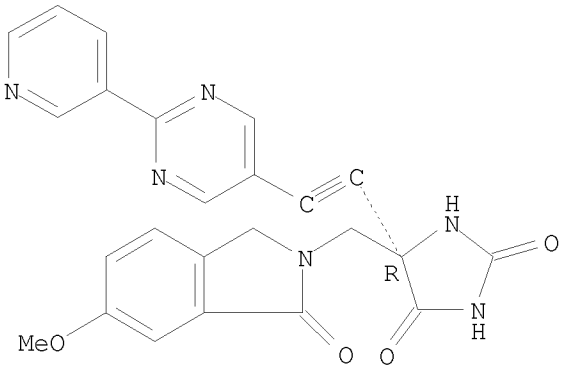
RN 944717-15-1 CAPLUS
CN 2,4(1H,3H)-Pyrimidinedione, 5-[2-[(4R)-4-[(1,3-dihydro-6-methoxy-1-oxo-2H-isoindol-2-yl)methyl]-2,5-dioxo-4-imidazolidinyl]ethynyl]-6-methyl- (CA INDEX NAME)

Absolute stereochemistry.



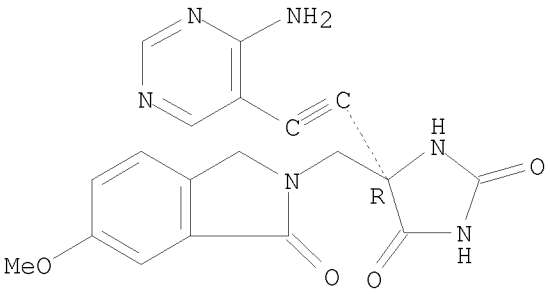
RN 944717-41-3 CAPLUS
CN 2,4-Imidazolidinedione, 5-[(1,3-dihydro-6-methoxy-1-oxo-2H-isoindol-2-yl)methyl]-5-[2-[2-(3-pyridinyl)-5-pyrimidinyl]ethynyl]-, (5R)- (CA INDEX NAME)

Absolute stereochemistry.



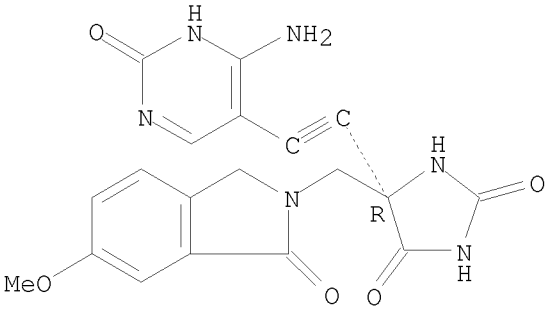
RN 944717-89-9 CAPLUS
CN 2,4-Imidazolidinedione, 5-[2-(4-amino-5-pyrimidinyl)ethynyl]-5-[(1,3-dihydro-6-methoxy-1-oxo-2H-isoindol-2-yl)methyl]-, (5R)- (CA INDEX NAME)

Absolute stereochemistry.



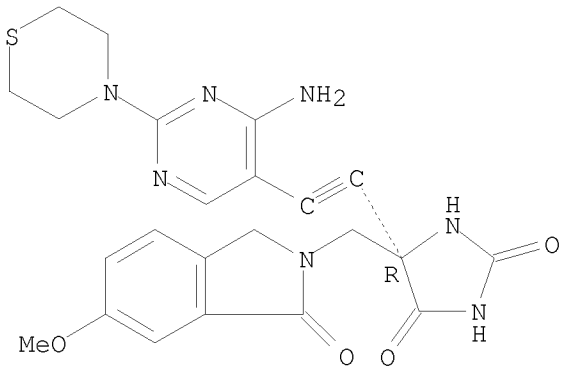
RN 944717-95-7 CAPLUS
CN 2,4-Imidazolidinedione, 5-[2-(4-amino-2,3-dihydro-2-oxo-5-pyrimidinyl)ethynyl]-5-[(1,3-dihydro-6-methoxy-1-oxo-2H-isoindol-2-yl)methyl]-, (5R)- (CA INDEX NAME)

Absolute stereochemistry.



RN 944718-00-7 CAPLUS
CN 2,4-Imidazolidinedione, 5-[2-[4-amino-2-(4-thiomorpholinyl)-5-pyrimidinyl]ethynyl]-5-[(1,3-dihydro-6-methoxy-1-oxo-2H-isoindol-2-yl)methyl]-, (5R)- (CA INDEX NAME)

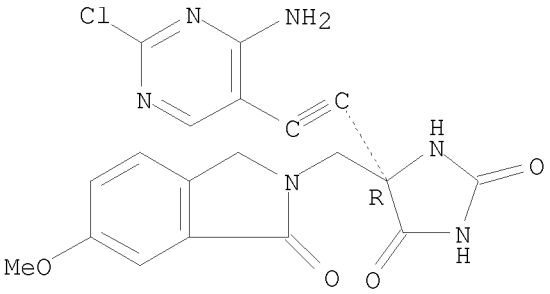
Absolute stereochemistry.



RN 944718-01-8 CAPLUS
CN 2,4-Imidazolidinedione, 5-[2-(4-amino-2-chloro-5-pyrimidinyl)ethynyl]-5-

[(1,3-dihydro-6-methoxy-1-oxo-2H-isoindol-2-yl)methyl]-, (5R)- (CA INDEX NAME)

Absolute stereochemistry.



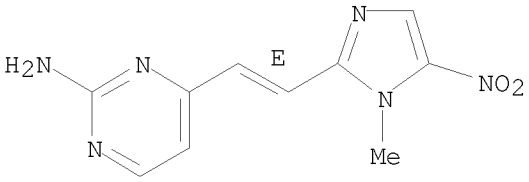
RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 7 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2007:769872 CAPLUS
DN 148:387155
TI Novel dosage form
IN Nadkarni, Sunil Sadanand; Vaya, Navin; Karan, Rajesh Singh; Gupta, Vinod Kumar
PA Torrent Pharmaceuticals Limited, India
SO Indian Pat. Appl., 96pp.
CODEN: INXXBQ
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI IN 2005MU01013	A	20070629	IN 2005-MU1013	20050826
PRAI IN 2005-MU1013		20050826		

AB A dosage form comprising of a high-dose, high-solubility active ingredient for modified release and a low-dose active ingredient for immediate release wherein the weight ratio of immediate-release active ingredient and modified-release active ingredient is from 1:10 to 1:15000 and the weight of modified-release active ingredient per unit is from 500 mg to 1500 mg. A process for preparing the dosage form is provided.
IT 62973-76-6, Azanidazole
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(novel dosage form containing modified-release and immediate-release active ingredients)
RN 62973-76-6 CAPLUS
CN 2-Pyrimidinamine, 4-[(1E)-2-(1-methyl-5-nitro-1H-imidazol-2-yl)ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.



L8 ANSWER 8 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2007:538389 CAPLUS
DN 146:521831
TI Preparation of six membered heteroaromatic, particularly pyrimidine and triazine, inhibitors targeting resistant kinase mutations for treating angiogenic and hematological associated disorders
IN Cao, Jianguo; Hood, John; Lohse, Dan; Mak, Chi Ching; Mc Pherson, Andrew; Noronha, Glenn; Pathak, Ved; Renick, Joel; Soll, Richard M.; Zeng, Binqi; Chow, Chun; Palanki, Moorthy; Dneprovskaia, Elena
PA Targegen, Inc., USA
SO PCT Int. Appl., 389pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2007056075	A2	20070518	WO 2006-US42838	20061031
	WO 2007056075	A3	20070920		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW				
	RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA				
	US 20070149508	A1	20070628	US 2006-591076	20061031
	US 20070161645	A1	20070712	US 2006-591252	20061031
PRAI	US 2005-733115P	P	20051102		

OS MARPAT 146:521831
AB The invention is related to the preparation of heteroaroms. I [L = C6H4-[X-M-[CH(R1)]p(CH2)q[CH(R2)]nG0R3R4]; X = O, CO, SO2, CH2; M = a bond, NH and derivs.; or X-M = a bond; R1, R2 = independently at each occurrence H, CF3, F, Cl, OH, NH2, (un)substituted aryl, alkyl, etc.; or R1-R2 = a bond, (CH2)a, (CH2)m-S-(CH2)a, (CH2)m-NR9-(CH2)a, etc.; m, n, p, q, a = independently 0-6; R9 = H, (un)substituted alk(en/yn)yl, etc.; G0 = N, O, H, CH; if G0 = N, then each R3, R4 = independently H, CF3, F, Cl, Br, I, OH, OMe, CN, OCF3, NH2, (un)substituted hydroxy/amino/alkyl, (hetero)aryl, or R3-R4 = (CH2)a, (CH2)m-S-(CH2)a, (CH2)a, (CH2)m-O-(CH2)a, etc.; if G0 = N; then R1-R9, or R1-R4, or R9-R4 or R3-R4 = independently (CH2)a, (CH2)m-S-(CH2)a, (CH2)m-O-(CH2)a, etc.; if G0 = O, R3 = H, CF3, F, Br, NH2, alkyl, aryl, etc., with no group R4; R1-R9 or R1-R3 or R9-R3 = independently (CH2)a, (CH2)m-S-(CH2)a, (CH2)a, (CH2)m-O-(CH2)a, etc.; if G0 = CH, R3, R4 = independently H, CF3, CN, (un)substituted amino/hydroxy/alkyl, etc.; or R3-R4 = (CHR9)m-(CHR9)a-(CHR9)p; (CHR9)m-S-(CHR9)a, (CHR9)m-O-(CHR9)a, etc.; A = (hetero)aryl; G = N, CH, CR; R = (un)substituted alkyl; Y = CH:CH, CH2CH2] as inhibitors targeting resistant kinase mutations. Thus, bromination of 3-amino-1,2,4-triazine, Pd-coupling of the bromide with [trans-2-(3-methoxyphenyl)ethenyl]boronic acid, amination of 4-bromo-N-[2-(pyrrolidin-1-yl)ethyl]benzenesulfonamide and demethylation gave triazine II. In a luminescent assay, pyrimidine III inhibited Abl and Abl(T3151) kinases with IC50 values of 25 nM and 240

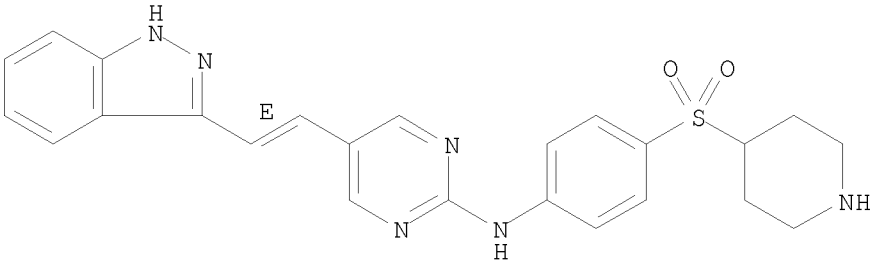
nM. I are useful for treating various angiogenic and hematol. associated disorders, such as myeloproliferative disorder in patients who do not respond to kinase-inhibition therapy that comprises administering approved medications (no data).

IT 937012-51-6P 937012-93-6P 937013-11-1P
937013-20-2P 937013-22-4P, 7-[(E)-2-[2-[[4-[(Piperidin-4-yl)sulfonyl]phenyl]amino]pyrimidin-5-yl]ethenyl]-5-(trifluoromethyl)-1H-benzimidazol-2-amine 937013-24-6P, 5-[(E)-2-[6-(Trifluoromethyl)-1H-benzo[d][1,2,3]triazol-4-yl]ethenyl]-N-[4-[(piperidin-4-yl)sulfonyl]phenyl]pyrimidin-2-amine 937013-25-7P, 5-[(E)-2-[6-(Trifluoromethyl)-1H-benzimidazol-4-yl]ethenyl]-N-[4-[(piperidin-4-yl)sulfonyl]phenyl]pyrimidin-2-amine 937013-26-8P, 5-[(E)-2-(1H-Benzo[d][1,2,3]triazol-5-yl)ethenyl]-N-[4-[(piperidin-4-yl)sulfonyl]phenyl]pyrimidin-2-amine 937013-28-0P
937013-30-4P 937013-32-6P 937013-34-8P
937013-71-3P, N-[4-[(1-Methylpiperidin-4-yl)sulfonyl]phenyl]-5-[(E)-2-(1H-indazol-4-yl)ethenyl]pyrimidin-2-amine 937013-72-4P
937013-74-6P 937013-76-8P 937013-85-9P,
5-[(E)-2-(1H-Indazol-4-yl)ethenyl]-N-[4-[(piperidin-4-yl)sulfonyl]phenyl]pyrimidin-2-amine hydrochloride 937013-90-6P
937013-91-7P 937013-98-4P 937013-99-5P
937014-81-8P, N-[4-[(Piperidin-4-yl)sulfonyl]phenyl]-5-[(E)-2-(1H-pyrrolo[2,3-b]pyridin-4-yl)ethenyl]pyrimidin-2-amine 937014-87-4P
, 5-[(E)-2-(1H-Indazol-4-yl)ethenyl]-N-[4-[[3-(pyrrolidin-1-yl)propyl]sulfonyl]phenyl]pyrimidin-2-amine 937014-92-1P,
6-[(E)-2-[2-[[4-[(Piperidin-4-yl)sulfonyl]phenyl]amino]pyrimidin-5-yl]ethenyl]-1H-benzimidazol-2-amine 937014-95-4P
937014-96-5P 937014-97-6P 937014-98-7P
937015-07-1P 937015-18-4P 937015-27-5P,
5-[(E)-2-(1H-Indazol-4-yl)ethenyl]-N-[3-(piperazin-1-yl)-4-[(piperazin-1-yl)sulfonyl]phenyl]pyrimidin-2-amine 937015-38-8P,
N-[2-(Dimethylamino)ethyl]-4-[[5-[(E)-2-(1H-indazol-4-yl)ethenyl]pyrimidin-2-yl]amino]-N-(piperidin-4-yl)benzenesulfonamide 937015-41-3P,
N-[4-[(4-Aminopiperidin-1-yl)sulfonyl]phenyl]-5-[(E)-2-(1H-indazol-4-yl)ethenyl]pyrimidin-2-amine 937015-47-9P, N-(2-Hydroxyethyl)-4-[[5-[(E)-2-(1H-indazol-4-yl)ethenyl]pyrimidin-2-yl]amino]-N-(piperidin-4-yl)benzenesulfonamide 937015-68-4P 937015-69-5P
937016-01-8P 937016-10-9P 937016-11-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of six membered heteroarom., particularly pyrimidine and triazine, inhibitors targeting resistant kinase mutations)

RN 937012-51-6 CAPLUS

CN 2-Pyrimidinamine, 5-[(1E)-2-(1H-indazol-3-yl)ethenyl]-N-[4-(4-piperidinylsulfonyl)phenyl]-, hydrochloride (1:1) (CA INDEX NAME)

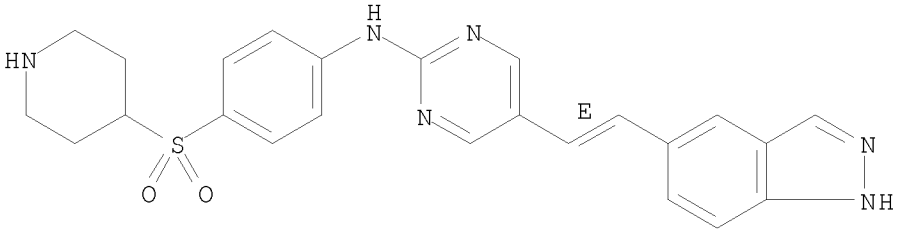
Double bond geometry as shown.



● HCl

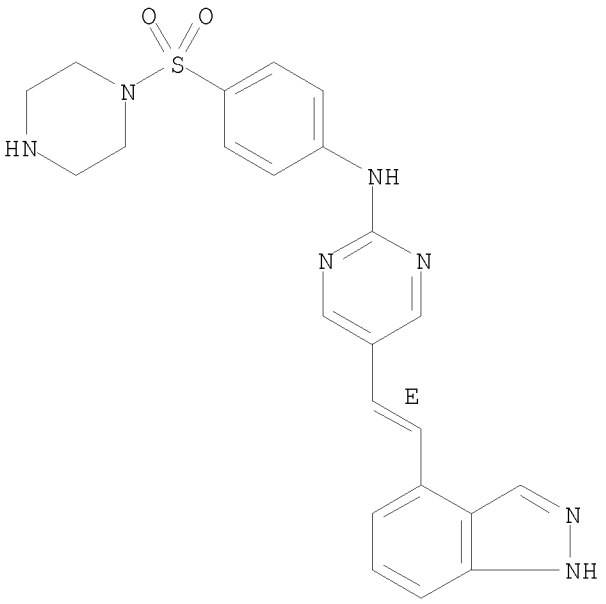
RN 937012-93-6 CAPLUS
CN 2-Pyrimidinamine, 5-[(1E)-2-(1H-indazol-5-yl)ethenyl]-N-[4-(4-piperidinylsulfonyl)phenyl]- (CA INDEX NAME)

Double bond geometry as shown.



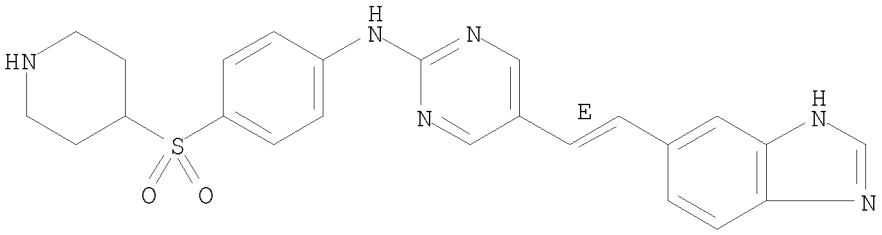
RN 937013-11-1 CAPLUS
CN 2-Pyrimidinamine, 5-[(1E)-2-(1H-indazol-4-yl)ethenyl]-N-[4-(1-piperazinylsulfonyl)phenyl]- (CA INDEX NAME)

Double bond geometry as shown.



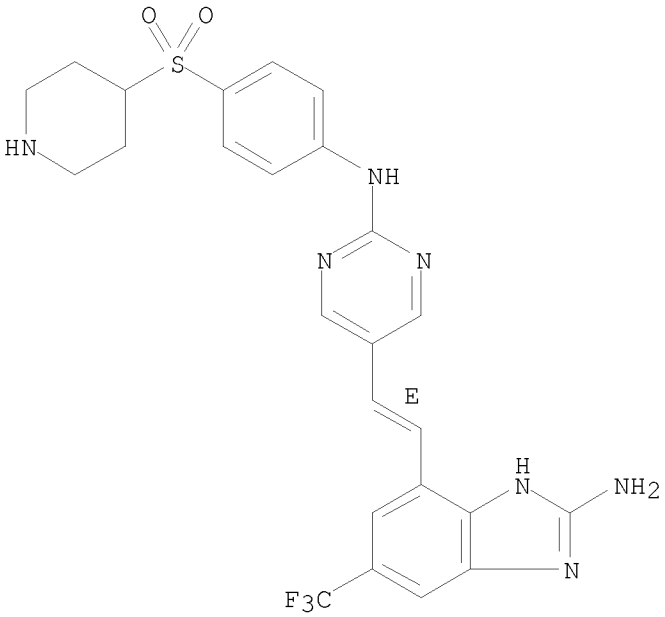
RN 937013-20-2 CAPLUS
CN 2-Pyrimidinamine, 5-[(1E)-2-(1H-benzimidazol-6-yl)ethenyl]-N-[4-(4-piperidinylsulfonyl)phenyl]- (CA INDEX NAME)

Double bond geometry as shown.



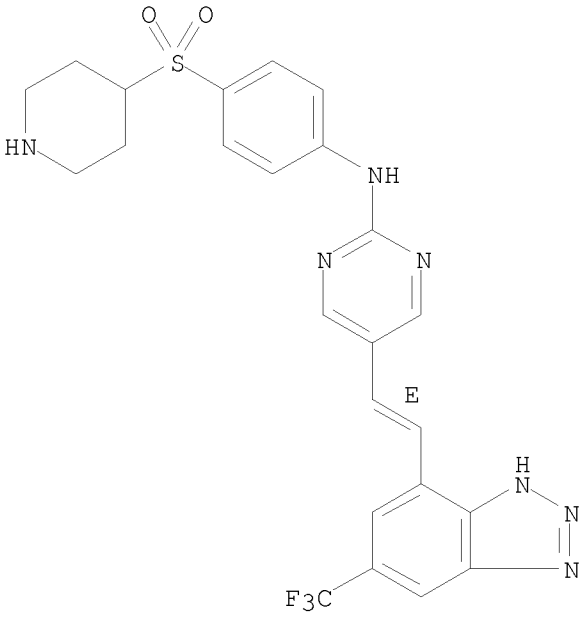
RN 937013-22-4 CAPLUS
CN 1H-Benzimidazol-2-amine, 7-[(1E)-2-[2-[[4-(4-piperidinylsulfonyl)phenyl]amino]-5-pyrimidinyl]ethenyl]-5-(trifluoromethyl)- (CA INDEX NAME)

Double bond geometry as shown.



RN 937013-24-6 CAPLUS
CN 2-Pyrimidinamine, N-[4-(4-piperidinylsulfonyl)phenyl]-5-[(1E)-2-[5-(trifluoromethyl)-1H-benzotriazol-7-yl]ethenyl]- (CA INDEX NAME)

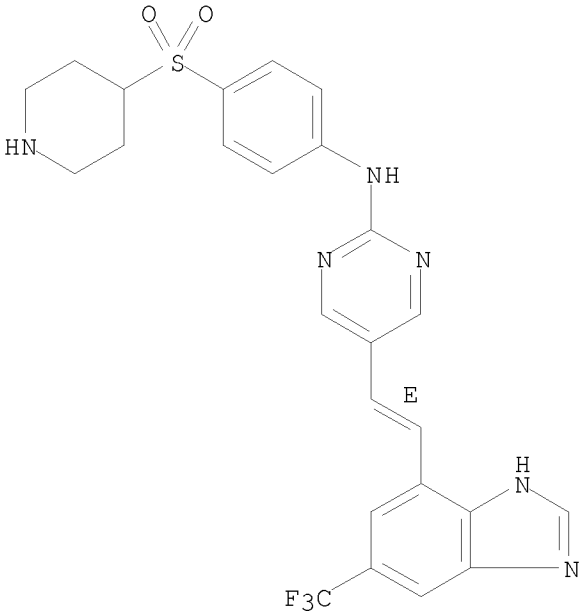
Double bond geometry as shown.



RN 937013-25-7 CAPLUS
CN 2-Pyrimidinamine, N-[4-(4-piperidinylsulfonyl)phenyl]-5-[(1E)-2-[5-

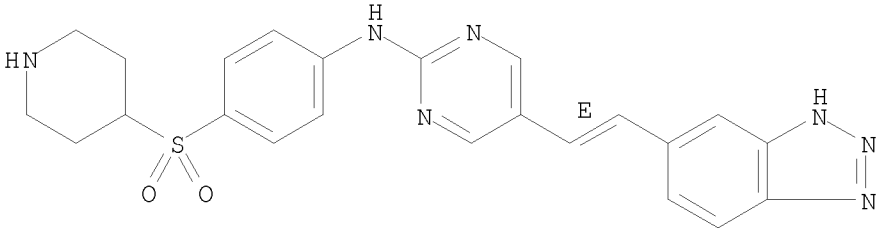
(trifluoromethyl)-1H-benzimidazol-7-yl]ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.



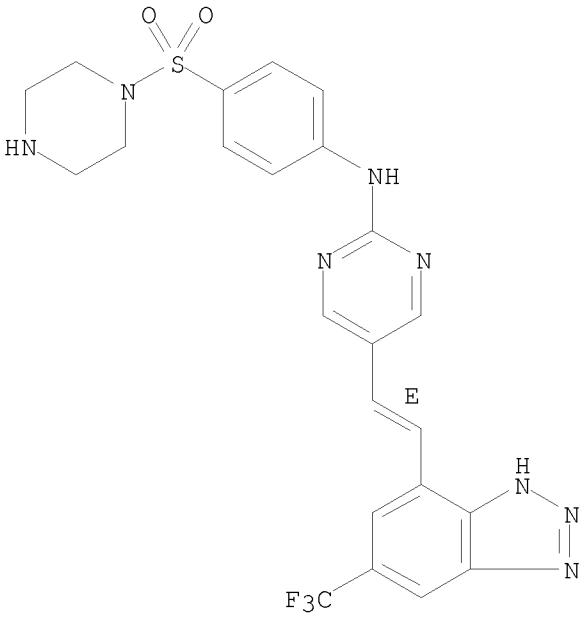
RN 937013-26-8 CAPLUS
CN 2-Pyrimidinamine, 5-[(1E)-2-(1H-benzotriazol-6-yl)ethenyl]-N-[4-(4-piperidinylsulfonyl)phenyl]- (CA INDEX NAME)

Double bond geometry as shown.



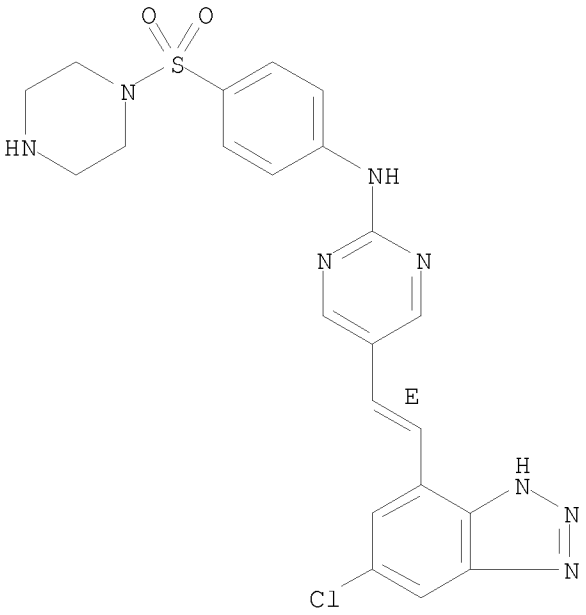
RN 937013-28-0 CAPLUS
CN 2-Pyrimidinamine, N-[4-(1-piperazinylsulfonyl)phenyl]-5-[(1E)-2-[5-(trifluoromethyl)-1H-benzotriazol-7-yl]ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.



RN 937013-30-4 CAPLUS
CN 2-Pyrimidinamine, 5-[(1E)-2-(5-chloro-1H-benzotriazol-7-yl)ethenyl]-N-[4-(1-piperazinylsulfonyl)phenyl]- (CA INDEX NAME)

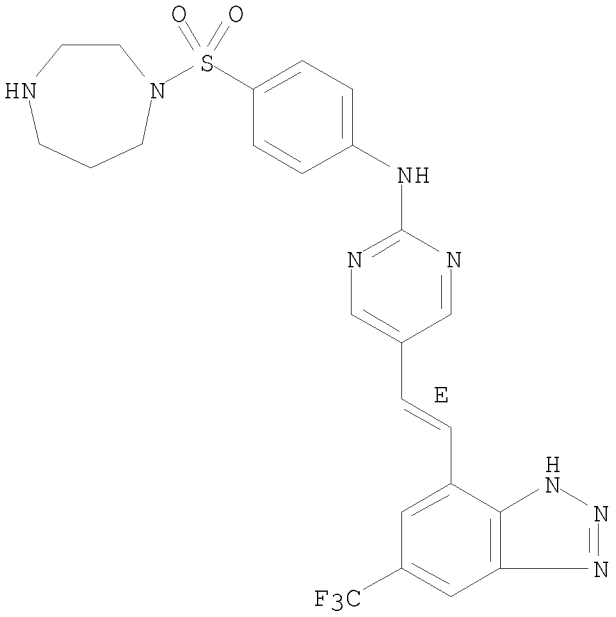
Double bond geometry as shown.



RN 937013-32-6 CAPLUS
CN 2-Pyrimidinamine, N-[4-[(hexahydro-1H-1,4-diazepin-1-yl)sulfonyl]phenyl]-5-[(1E)-2-[5-(trifluoromethyl)-1H-benzotriazol-7-yl]ethenyl]- (CA INDEX

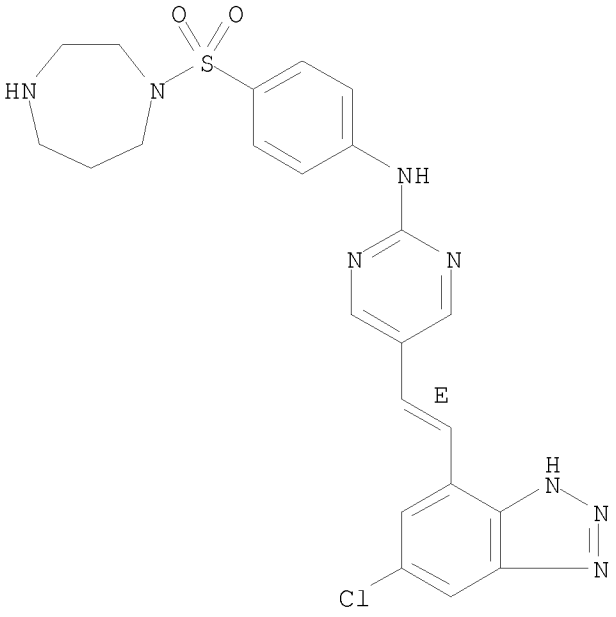
NAME)

Double bond geometry as shown.



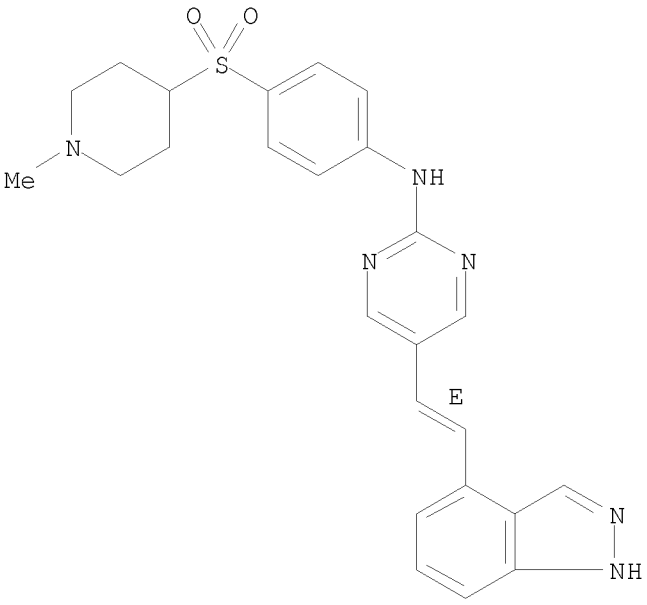
RN 937013-34-8 CAPLUS
CN 2-Pyrimidinamine, 5-[(1E)-2-(5-chloro-1H-benzotriazol-7-yl)ethenyl]-N-[4-[(hexahydro-1H-1,4-diazepin-1-yl)sulfonyl]phenyl]- (CA INDEX NAME)

Double bond geometry as shown.



RN 937013-71-3 CAPLUS
CN 2-Pyrimidinamine, 5-[(1E)-2-(1H-indazol-4-yl)ethenyl]-N-[4-[(1-methyl-4-piperidinyl)sulfonyl]phenyl]- (CA INDEX NAME)

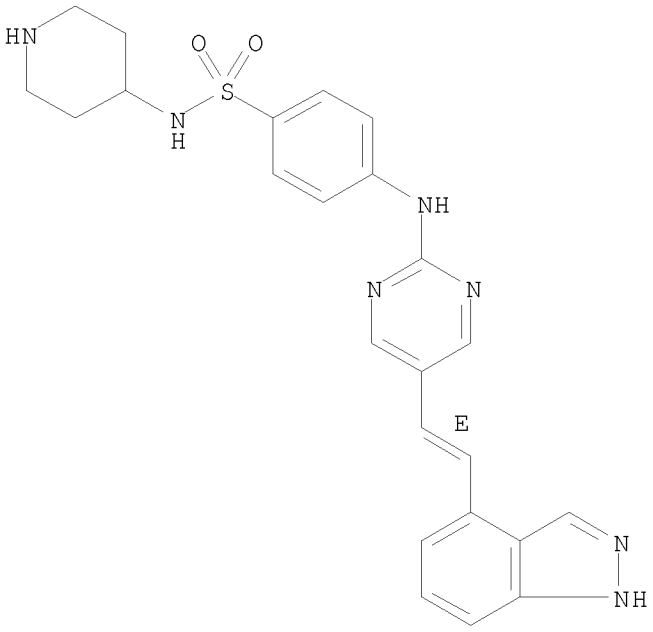
Double bond geometry as shown.



RN 937013-72-4 CAPLUS
CN Benzenesulfonamide, 4-[[5-[(1E)-2-(1H-indazol-4-yl)ethenyl]-2-pyrimidinyl]amino]-N-4-piperidinyl-, hydrochloride (1:?) (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A

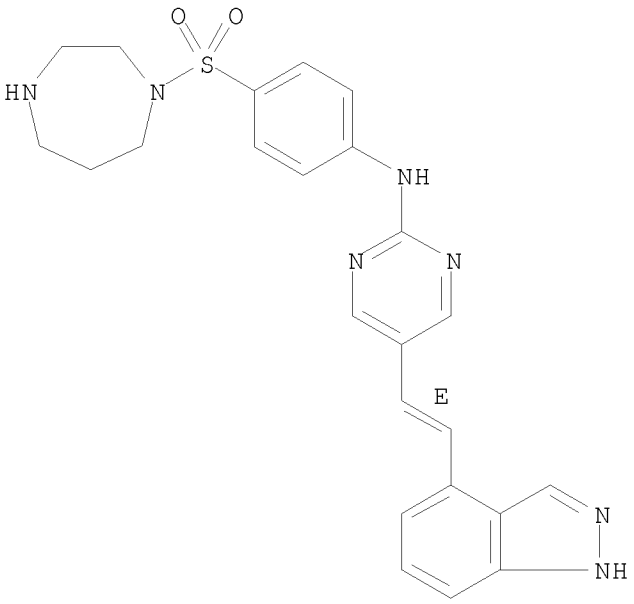


PAGE 2-A

●x HCl

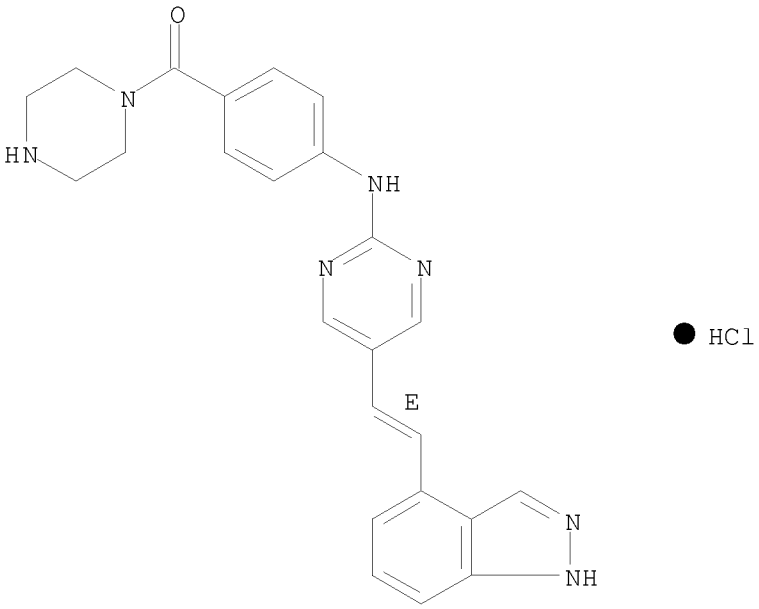
RN 937013-74-6 CAPLUS
CN 2-Pyrimidinamine, N-[4-[(hexahydro-1H-1,4-diazepin-1-yl)sulfonyl]phenyl]-5-[(1E)-2-(1H-indazol-4-yl)ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.



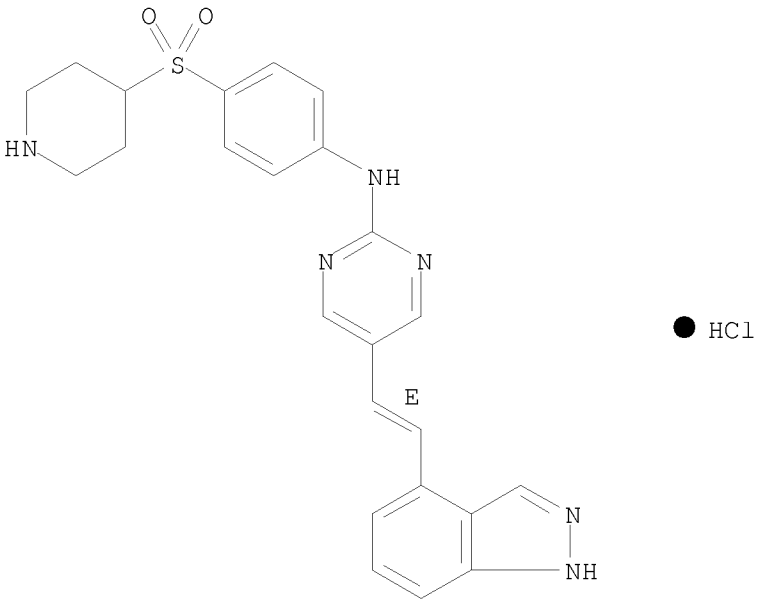
RN 937013-76-8 CAPLUS
CN Methanone, [4-[[5-[(1E)-2-(1H-indazol-4-yl)ethenyl]-2-pyrimidinyl]amino]phenyl]-1-piperazinyl-, hydrochloride (1:1) (CA INDEX NAME)

Double bond geometry as shown.



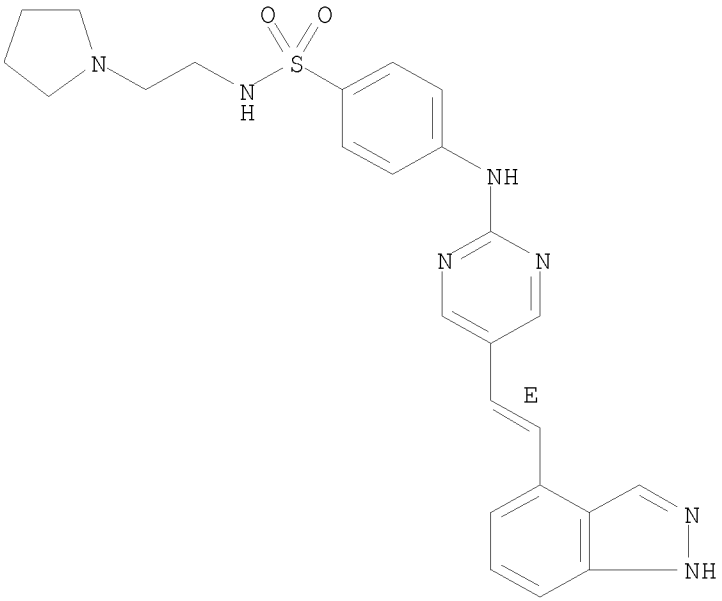
RN 937013-85-9 CAPLUS
CN 2-Pyrimidinamine, 5-[(1E)-2-(1H-indazol-4-yl)ethenyl]-N-[4-(4-piperidinylsulfonyl)phenyl]-, hydrochloride (1:1) (CA INDEX NAME)

Double bond geometry as shown.



RN 937013-90-6 CAPLUS
CN Benzenesulfonamide, 4-[[5-[(1E)-2-(1H-indazol-4-yl)ethenyl]-2-pyrimidinyl]amino]-N-[2-(1-pyrrolidinyl)ethyl]- (CA INDEX NAME)

Double bond geometry as shown.



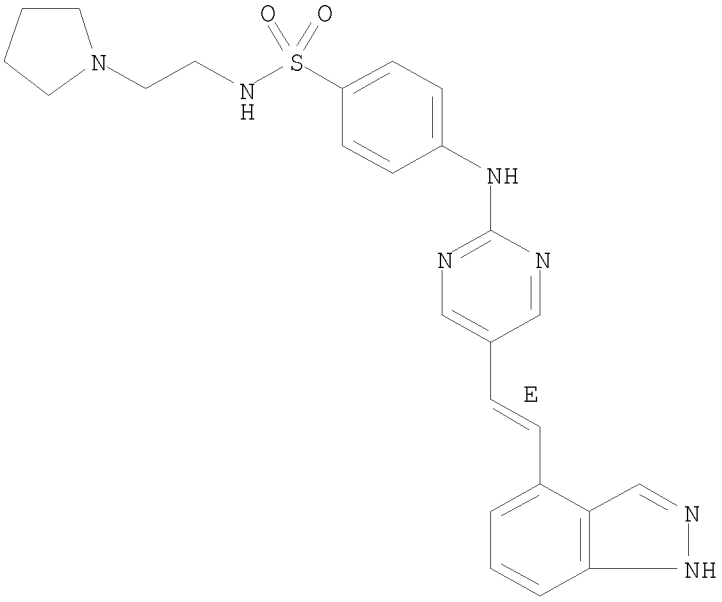
RN 937013-91-7 CAPLUS
CN Benzenesulfonamide, 4-[[5-[(1E)-2-(1H-indazol-4-yl)ethenyl]-2-

pyrimidinyl]amino]-N-[2-(1-pyrrolidinyl)ethyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

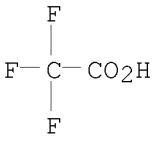
CRN 937013-90-6
CMF C25 H27 N7 O2 S

Double bond geometry as shown.



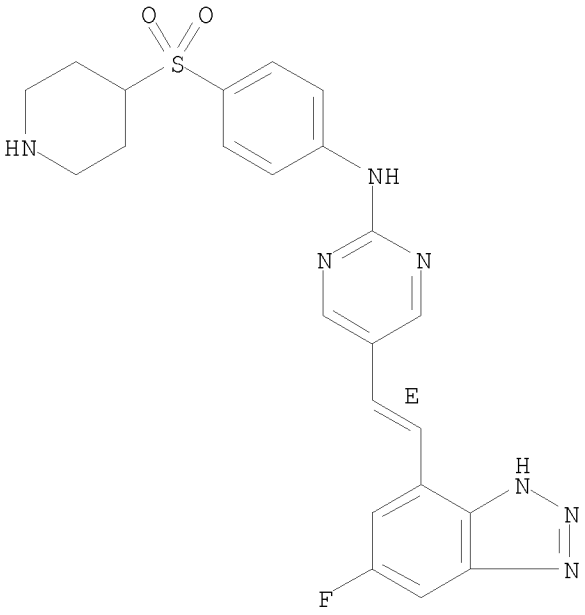
CM 2

CRN 76-05-1
CMF C2 H F3 O2



RN 937013-98-4 CAPLUS
CN 2-Pyrimidinamine, 5-[(1E)-2-(5-fluoro-1H-benzotriazol-7-yl)ethenyl]-N-[4-(4-piperidinylsulfonyl)phenyl]- (CA INDEX NAME)

Double bond geometry as shown.

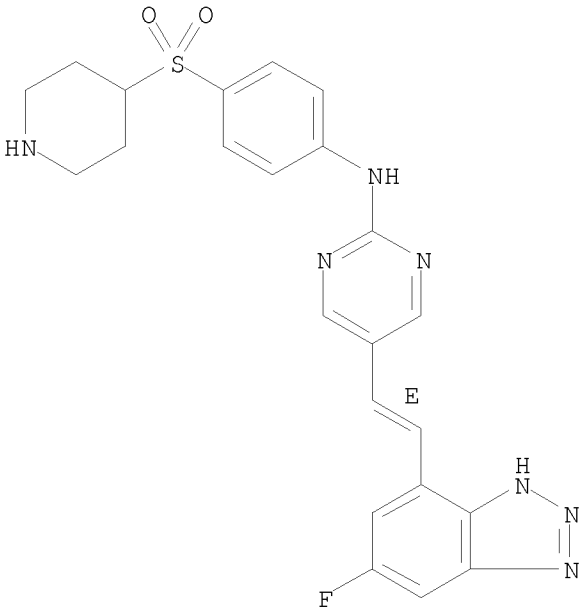


RN 937013-99-5 CAPLUS
CN 2-Pyrimidinamine, 5-[(1E)-2-(5-fluoro-1H-benzotriazol-7-yl)ethenyl]-N-[4-(4-piperidinylsulfonyl)phenyl]-, 2,2,2-trifluoroacetate (1:?) (CA INDEX NAME)

CM 1

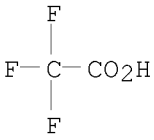
CRN 937013-98-4
CMF C23 H22 F N7 O2 S

Double bond geometry as shown.



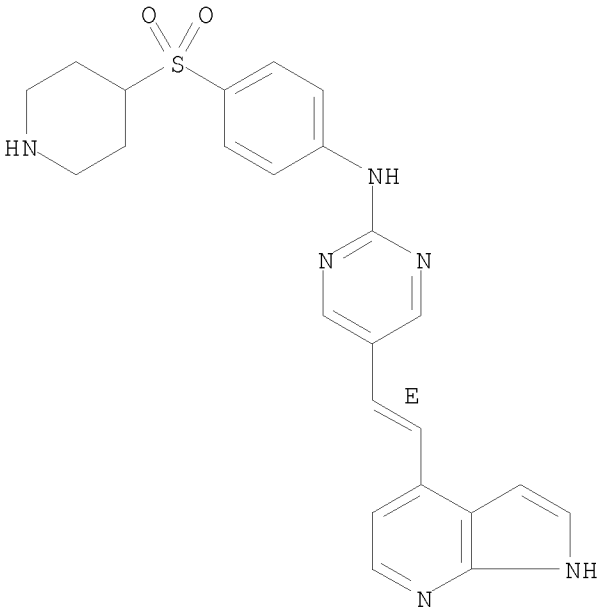
CM 2

CRN 76-05-1
CMF C2 H F3 O2



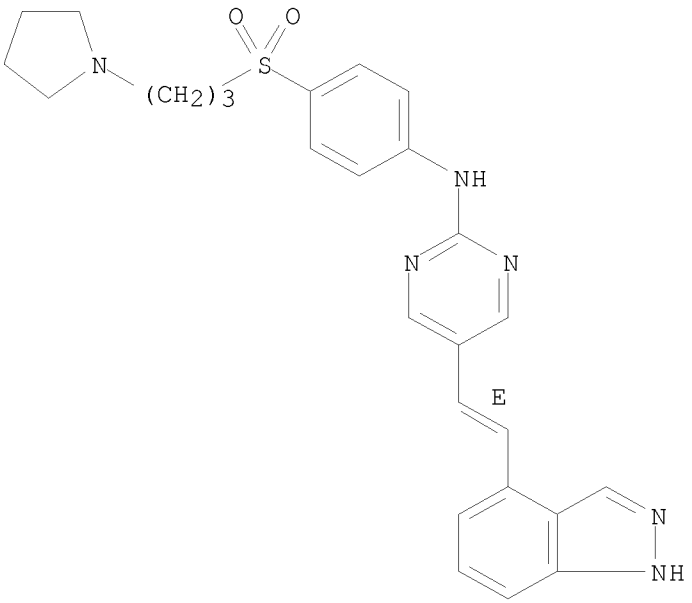
RN 937014-81-8 CAPLUS
CN 2-Pyrimidinamine, N-[4-(4-piperidinylsulfonyl)phenyl]-5-[(1E)-2-(1H-pyrrolo[2,3-b]pyridin-4-yl)ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.



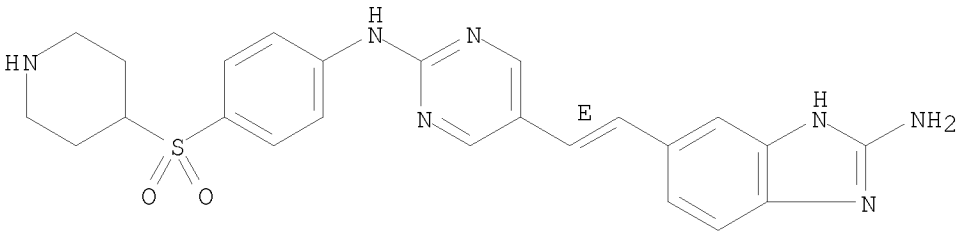
RN 937014-87-4 CAPLUS
CN 2-Pyrimidinamine, 5-[(1E)-2-(1H-indazol-4-yl)ethenyl]-N-[4-[[3-(1-pyrrolidinyl)propyl]sulfonyl]phenyl]- (CA INDEX NAME)

Double bond geometry as shown.



RN 937014-92-1 CAPLUS
CN 1H-Benzimidazol-2-amine, 6-[(1E)-2-[2-[[4-(4-piperidinylsulfonyl)phenyl]amino]-5-pyrimidinyl]ethenyl]- (CA INDEX NAME)

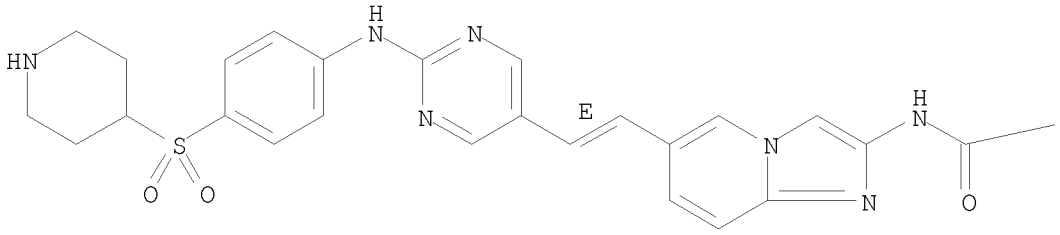
Double bond geometry as shown.



RN 937014-95-4 CAPLUS
CN Acetamide, 2,2,2-trifluoro-N-[6-[(1E)-2-[2-[[4-(4-piperidinylsulfonyl)phenyl]amino]-5-pyrimidinyl]ethenyl]imidazo[1,2-a]pyridin-2-yl]- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



PAGE 1-B

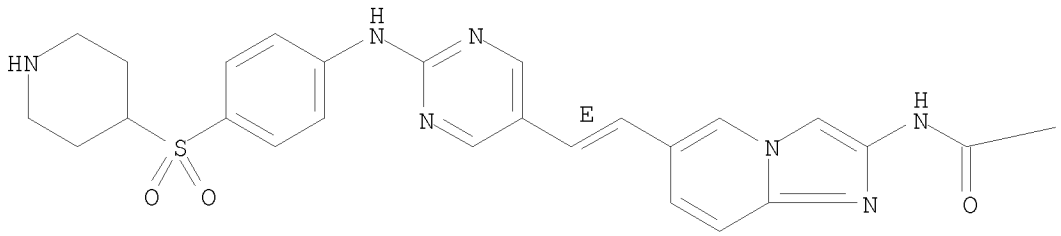
RN 937014-96-5 CAPLUS
CN Acetamide, 2,2,2-trifluoro-N-[6-[(1E)-2-[2-[[4-(4-piperidinylsulfonyl)phenyl]amino]-5-pyrimidinyl]ethenyl]imidazo[1,2-a]pyridin-2-yl]-, 2,2,2-trifluoroacetate (1:?) (CA INDEX NAME)

CM 1

CRN 937014-95-4
CMF C26 H24 F3 N7 O3 S

Double bond geometry as shown.

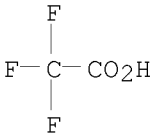
PAGE 1-A



PAGE 1-B

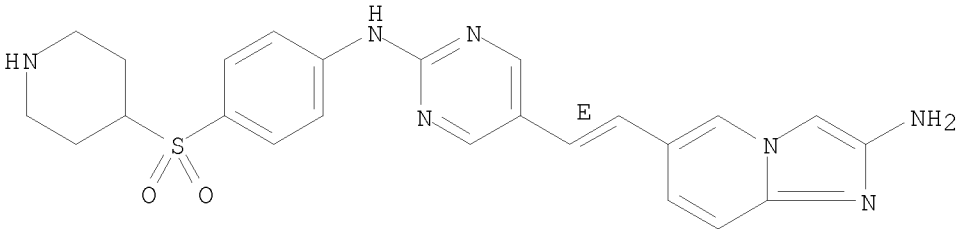
CM 2

CRN 76-05-1
CMF C2 H F3 O2



RN 937014-97-6 CAPLUS
CN Imidazo[1,2-a]pyridin-2-amine, 6-[(1E)-2-[2-[[4-(4-piperidinylsulfonyl)phenyl]amino]-5-pyrimidinyl]ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.

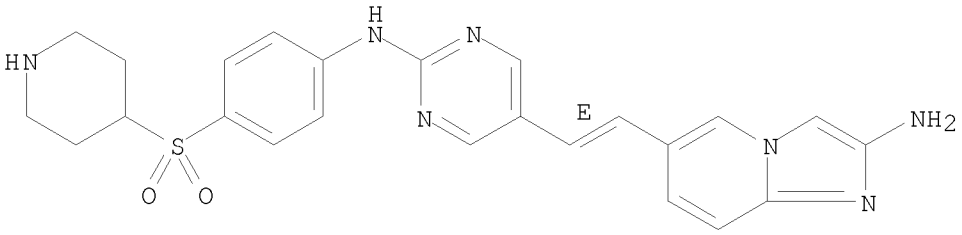


RN 937014-98-7 CAPLUS
CN Imidazo[1,2-a]pyridin-2-amine, 6-[(1E)-2-[2-[[4-(4-piperidinylsulfonyl)phenyl]amino]-5-pyrimidinyl]ethenyl]-, 2,2,2-trifluoroacetate (1:?) (CA INDEX NAME)

CM 1

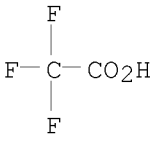
CRN 937014-97-6
CMF C24 H25 N7 O2 S

Double bond geometry as shown.



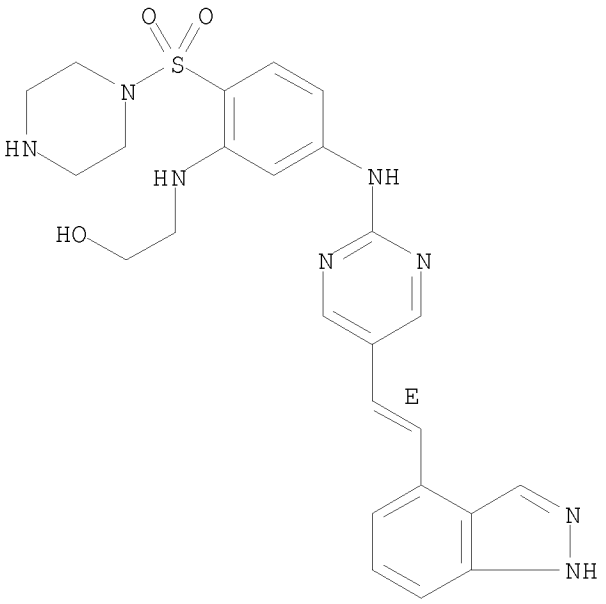
CM 2

CRN 76-05-1
CMF C2 H F3 O2



RN 937015-07-1 CAPLUS
CN Ethanol, 2-[[5-[[5-[(1E)-2-(1H-indazol-4-yl)ethenyl]-2-pyrimidinyl]amino]-2-(1-piperazinylsulfonyl)phenyl]amino]- (CA INDEX NAME)

Double bond geometry as shown.

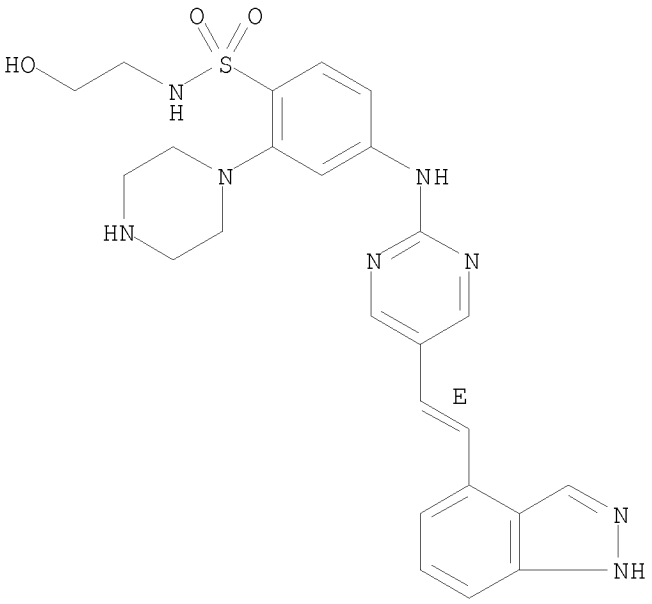


RN 937015-18-4 CAPLUS
CN Benzenesulfonamide, N-(2-hydroxyethyl)-4-[[5-[(1E)-2-(1H-indazol-4-yl)ethenyl]-2-pyrimidinyl]amino]-2-(1-piperazinyl)-, 2,2,2-trifluoroacetate (1:?) (CA INDEX NAME)

CM 1

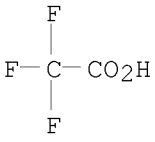
CRN 937015-17-3
CMF C25 H28 N8 O3 S

Double bond geometry as shown.



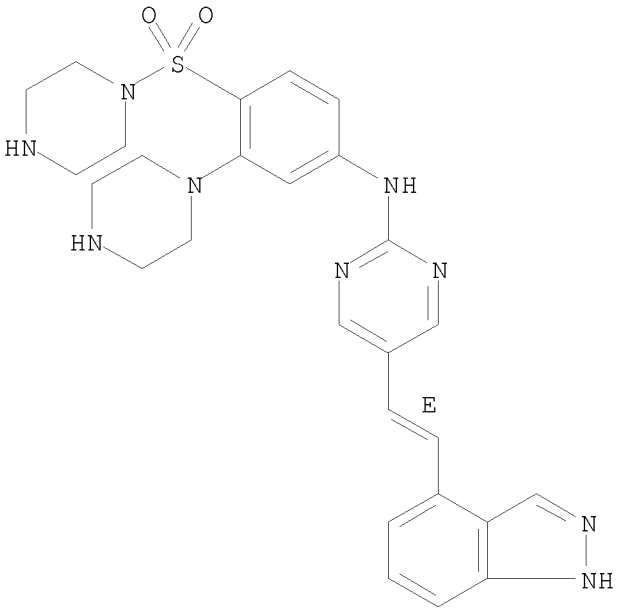
CM 2

CRN 76-05-1
CMF C2 H F3 O2



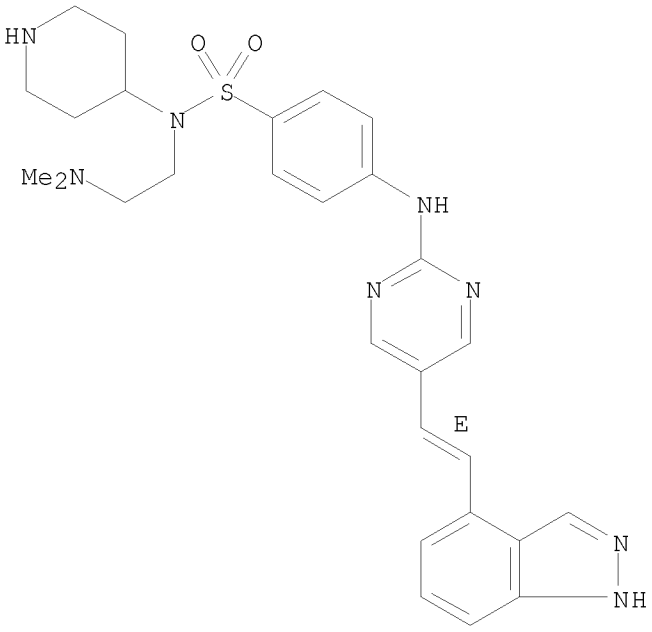
RN 937015-27-5 CAPLUS
CN 2-Pyrimidinamine, 5-[(1E)-2-(1H-indazol-4-yl)ethenyl]-N-[3-(1-piperazinyl)-4-(1-piperazinylsulfonyl)phenyl]- (CA INDEX NAME)

Double bond geometry as shown.



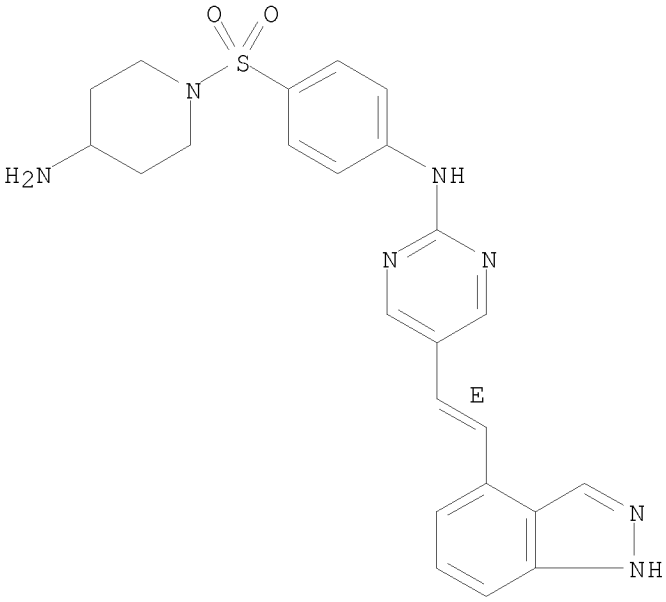
RN 937015-38-8 CAPLUS
CN Benzenesulfonamide, N-[2-(dimethylamino)ethyl]-4-[[5-[(1E)-2-(1H-indazol-4-yl)ethenyl]-2-pyrimidinyl]amino]-N-4-piperidinyl- (CA INDEX NAME)

Double bond geometry as shown.



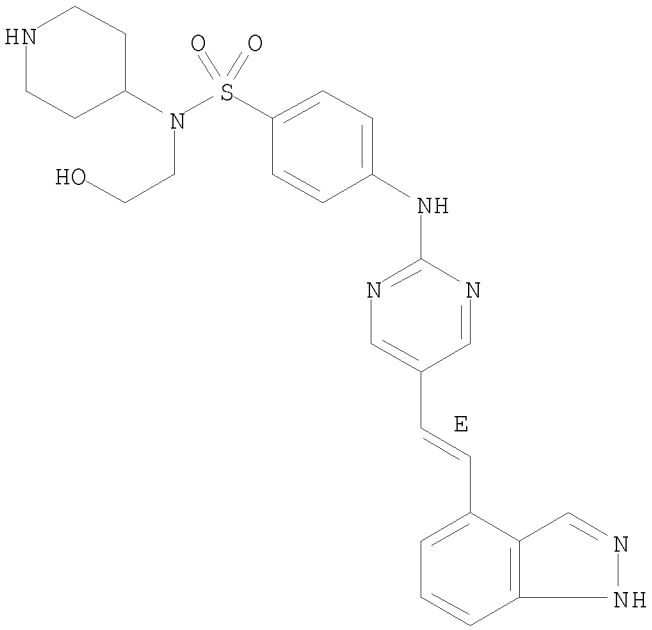
RN 937015-41-3 CAPLUS
CN 2-Pyrimidinamine, N-[4-[(4-amino-1-piperidinyl)sulfonyl]phenyl]-5-[(1E)-2-(1H-indazol-4-yl)ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.



RN 937015-47-9 CAPLUS
CN Benzenesulfonamide, N-(2-hydroxyethyl)-4-[[5-[(1E)-2-(1H-indazol-4-yl)ethenyl]-2-pyrimidinyl]amino]-N-4-piperidinyl- (CA INDEX NAME)

Double bond geometry as shown.



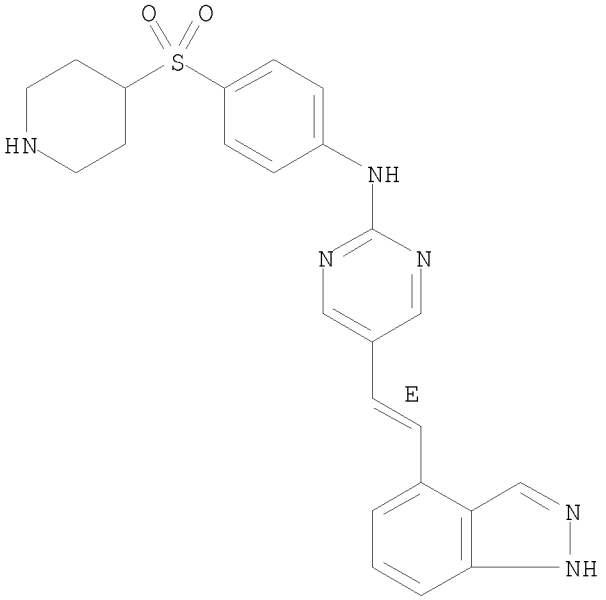
RN 937015-68-4 CAPLUS

CN 2-Pyrimidinamine, 5-[(1E)-2-(1H-indazol-4-yl)ethenyl]-N-[4-(4-piperidinylsulfonyl)phenyl]-, 2,2,2-trifluoroacetate (1:?) (CA INDEX NAME)

CM 1

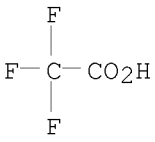
CRN 937015-67-3
CMF C24 H24 N6 O2 S

Double bond geometry as shown.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

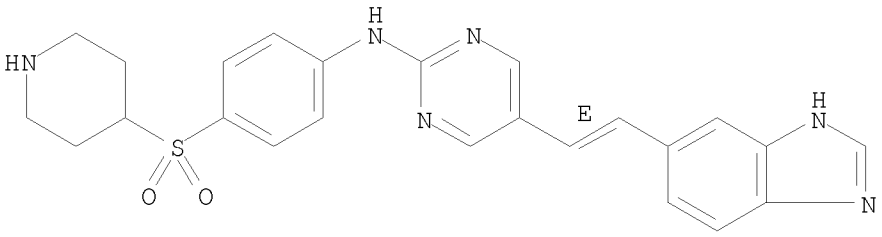


RN 937015-69-5 CAPLUS
CN Methanesulfonic acid, 1,1,1-trifluoro-, compd. with 5-[(1E)-2-(1H-benzimidazol-6-yl)ethenyl]-N-[4-(4-piperidinylsulfonyl)phenyl]-2-pyrimidinamine (1:?) (CA INDEX NAME)

CM 1

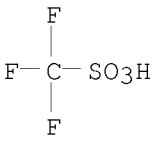
CRN 937013-20-2
CMF C24 H24 N6 O2 S

Double bond geometry as shown.



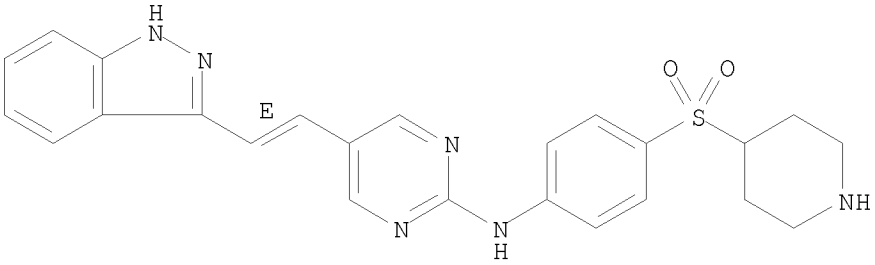
CM 2

CRN 1493-13-6
CMF C H F3 O3 S



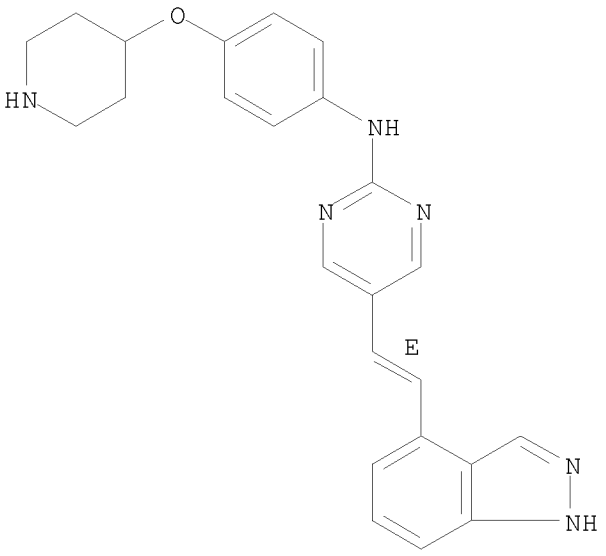
RN 937016-01-8 CAPLUS
CN 2-Pyrimidinamine, 5-[(1E)-2-(1H-indazol-3-yl)ethenyl]-N-[4-(4-piperidinylsulfonyl)phenyl]- (CA INDEX NAME)

Double bond geometry as shown.



RN 937016-10-9 CAPLUS
CN 2-Pyrimidinamine, 5-[(1E)-2-(1H-indazol-4-yl)ethenyl]-N-[4-(4-piperidinyloxy)phenyl]- (CA INDEX NAME)

Double bond geometry as shown.

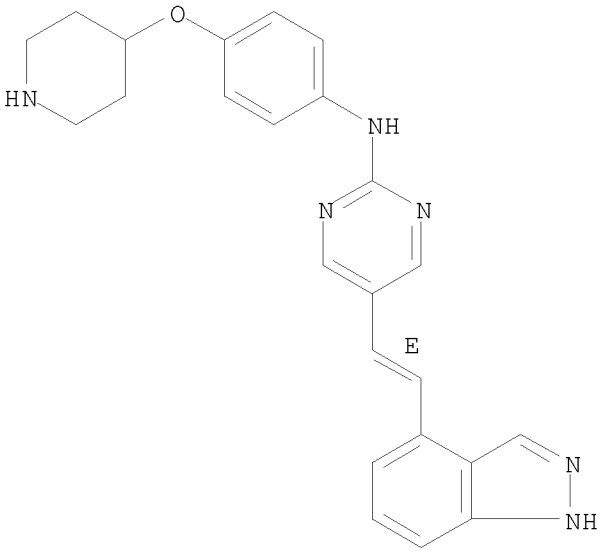


RN 937016-11-0 CAPLUS
CN 2-Pyrimidinamine, 5-[(1E)-2-(1H-indazol-4-yl)ethenyl]-N-[4-(4-piperidinyloxy)phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

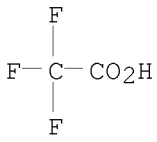
CRN 937016-10-9
CMF C24 H24 N6 O

Double bond geometry as shown.



CM 2

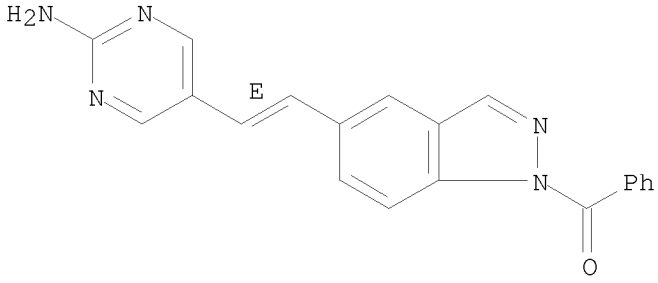
CRN 76-05-1
CMF C2 H F3 O2



IT 937012-92-5P 937013-73-5P 937013-84-8P,
tert-Butyl 4-[[4-[[5-[(E)-2-(1H-indazol-4-yl)ethenyl]pyrimidin-2-yl]amino]phenyl]sulfonyl]piperidine-1-carboxylate 937013-97-3P,
tert-Butyl 4-[[4-[[5-[(E)-2-(6-fluoro-1H-benzo[d][1,2,3]triazol-4-yl)ethenyl]pyrimidin-2-yl]amino]phenyl]sulfonyl]piperidine-1-carboxylate
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of six membered heteroarom., particularly pyrimidine and triazine, inhibitors targeting resistant kinase mutations)

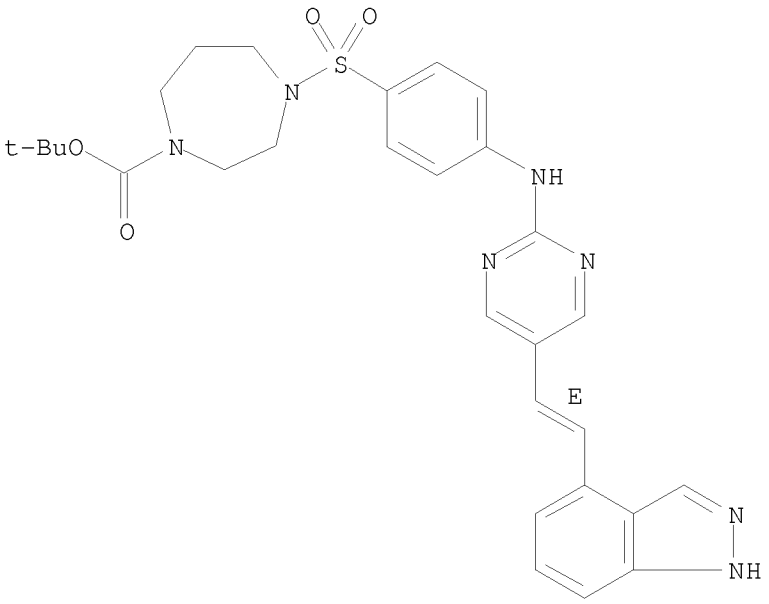
RN 937012-92-5 CAPLUS
CN Methanone, [5-[(1E)-2-(2-amino-5-pyrimidinyl)ethenyl]-1H-indazol-1-yl]phenyl- (CA INDEX NAME)

Double bond geometry as shown.



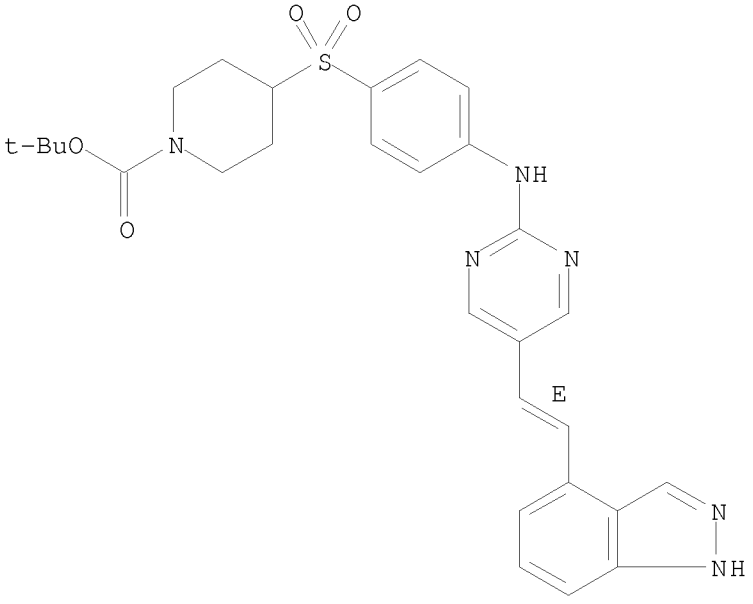
RN 937013-73-5 CAPLUS
CN 1H-1,4-Diazepine-1-carboxylic acid, hexahydro-4-[[4-[[5-[(1E)-2-(1H-indazol-4-yl)ethenyl]-2-pyrimidinyl]amino]phenyl]sulfonyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Double bond geometry as shown.



RN 937013-84-8 CAPLUS
CN 1-Piperidinecarboxylic acid, 4-[[4-[[5-[(1E)-2-(1H-indazol-4-yl)ethenyl]-2-pyrimidinyl]amino]phenyl]sulfonyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

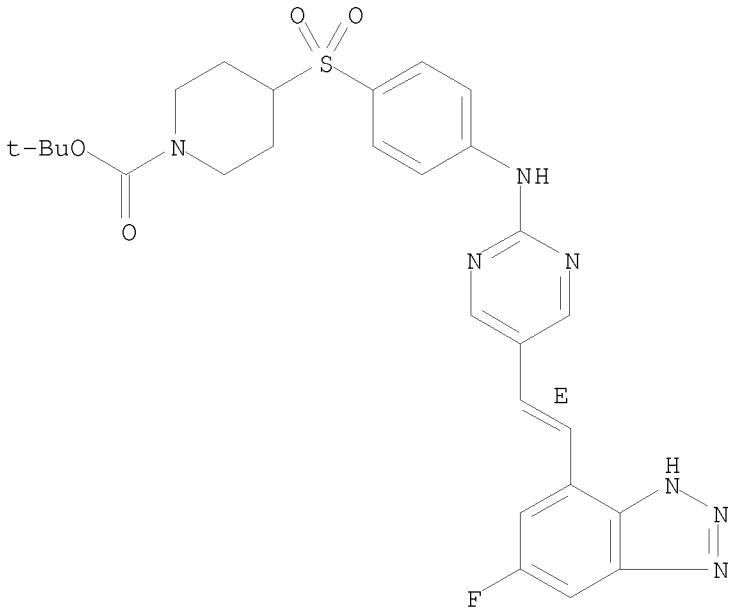
Double bond geometry as shown.



RN 937013-97-3 CAPLUS
CN 1-Piperidinecarboxylic acid, 4-[[4-[[5-[(1E)-2-(5-fluoro-1H-benzotriazol-7-yl)ethenyl]-2-pyrimidinyl]amino]phenyl]sulfonyl]-, 1,1-dimethylethyl ester

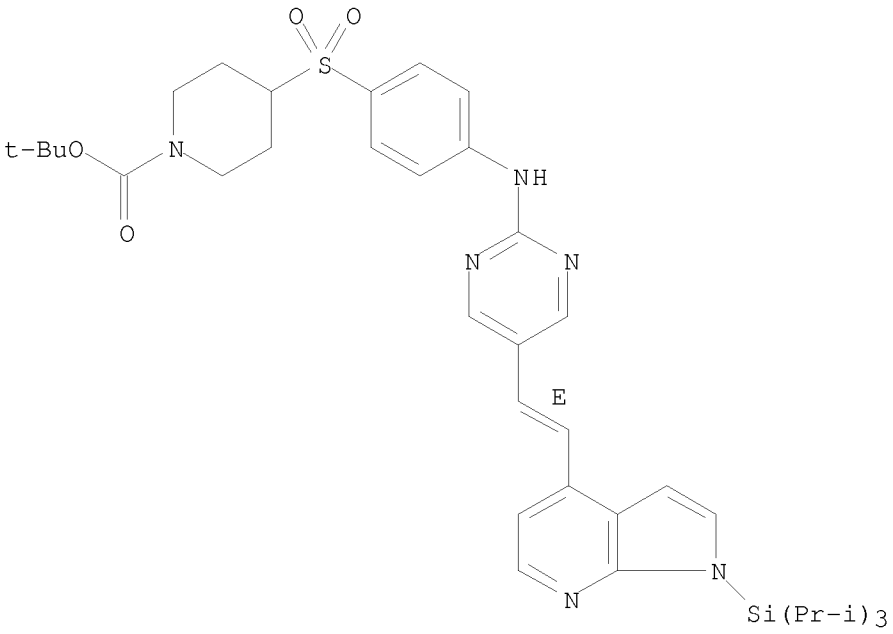
(CA INDEX NAME)

Double bond geometry as shown.



IT 937014-82-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of six membered heteroarom., particularly pyrimidine and triazine, inhibitors targeting resistant kinase mutations)
RN 937014-82-9 CAPLUS
CN 1-Piperidinecarboxylic acid, 4-[[4-[[5-[(1E)-2-[1-[tris(1-methylethyl)silyl]-1H-pyrrolo[2,3-b]pyridin-4-yl]ethenyl]-2-pyrimidinyl]amino]phenyl]sulfonyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Double bond geometry as shown.


O
O
S
t-BuO
N
NH
O
N
N
E
N
N
Si(Pr-i)3

L8 ANSWER 9 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2007:486155 CAPLUS
DN 146:482054
TI Thiazolyl derivatives as mGluR5 antagonists and their preparation and methods for their use
IN Cosford, Nicholas D.; Seiders, Thomas J.; Payne, Joseph; Roppe, Jeffrey R.; Huang, Dehua; Smith, Nicholas D.; Poon, Steve F.; King, Chris; Eastman, Brian W.; Wang, Bowei; Arruda, Jeannie M.; Vernier, Jean-Michel; Zhao, Xiumin
PA Merck & Co., Inc., USA
SO PCT Int. Appl., 58pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2007050050	A2	20070503	WO 2005-US35921	20051006
	WO 2007050050	A3	20080207		
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	RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA				
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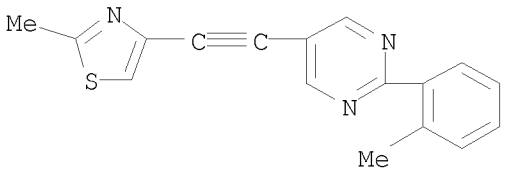
	AU 2005336513	A1	20070517	AU 2005-336513	20051006
	EP 1893608	A2	20080305	EP 2005-858618	20051006
	R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR				
	JP 2008516004	T	20080515	JP 2007-543041	20051006
	IN 2007CN01215	A	20070831	IN 2007-CN1215	20070323
PRAI	US 2004-616805P	P	20041007		
	WO 2005-US35921	W	20051006		

OS MARPAT 146:482054
AB The identification of a unique series of compds. of formula I, which possesses special advantages in terms of drug-like properties due to their possessing advantageous properties in terms of potency and/or pharmacokinetic and/or selectivity and/or in vivo receptor occupancy properties. Compds. of formula I wherein Z is C or N; when Z is N, X is absent; X is H; and Y is (un)substituted (hetero)aryl, amino, alkoxy, alkylthio, etc.; or Y is H; and X is (un)substituted (hetero)aryl, halo, cycloalkyl, alkenyl, amino, etc.; and their radioisotopes and pharmaceutically acceptable salts thereof are claimed. Specifically, the selection of a 1,3-thiazol-2-yl ring member linked by an ethynylene to the 3 position of a pyridyl ring or the 5 position of a pyrimidinyl ring, wherein the ring is substituted with selected substituents, results in a compound having superior drug-like properties. The invention includes pharmaceutically acceptable salt forms of these heterocyclic compds., in particular chloride salts and trifluoroacetate salts. Example compound II was prepared by cross-coupling of 2-chloro-5-[(2-methyl-1,3-thiazol-4-

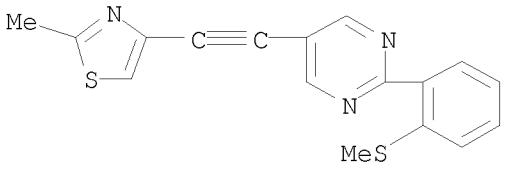
yl)ethynyl]pyridine with 2-fluorophenylboronic acid. All the invention compds. were evaluated for their mGluR5 antagonistic activity. From the assay, it was determined that compound II exhibited a Ki value of 2.0 nM.

IT 935684-71-2P 935684-72-3P 935684-73-4P
935684-74-5P 935684-79-0P 935684-81-4P
935684-84-7P 935684-88-1P 935684-91-6P
935685-61-3P 935685-63-5P 935685-65-7P
935685-67-9P 935685-69-1P 935685-71-5P
935685-72-6P 935685-74-8P 935685-76-0P
935685-77-1P 935685-79-3P 935685-81-7P
935685-83-9P 935685-85-1P 935685-86-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of (thiazolylethynyl)pyridines and -pyrimidines as mGluR5 antagonists)

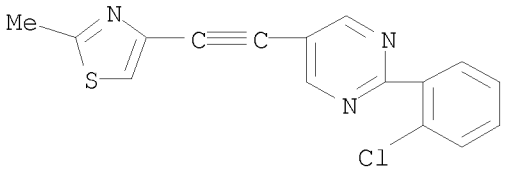
RN 935684-71-2 CAPLUS
CN Pyrimidine, 2-(2-methylphenyl)-5-[2-(2-methyl-4-thiazolyl)ethynyl]- (CA INDEX NAME)



RN 935684-72-3 CAPLUS
CN Pyrimidine, 5-[2-(2-methyl-4-thiazolyl)ethynyl]-2-[2-(methylthio)phenyl]- (CA INDEX NAME)

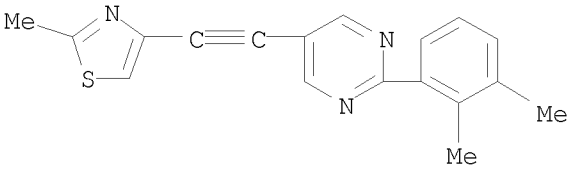


RN 935684-73-4 CAPLUS
CN Pyrimidine, 2-(2-chlorophenyl)-5-[2-(2-methyl-4-thiazolyl)ethynyl]- (CA INDEX NAME)

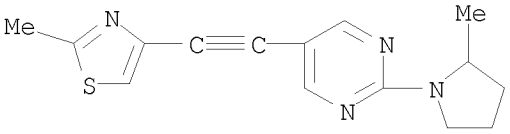


RN 935684-74-5 CAPLUS
CN Pyrimidine, 2-(2,3-dimethylphenyl)-5-[2-(2-methyl-4-thiazolyl)ethynyl]-

(CA INDEX NAME)



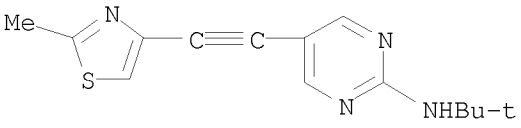
RN 935684-79-0 CAPLUS
CN Pyrimidine, 2-(2-methyl-1-pyrrolidinyl)-5-[2-(2-methyl-4-thiazolyl)ethynyl]- (CA INDEX NAME)



RN 935684-81-4 CAPLUS
CN 2-Pyrimidinamine, N-(1,1-dimethylethyl)-5-[2-(2-methyl-4-thiazolyl)ethynyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

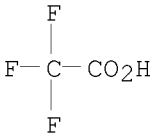
CM 1

CRN 935684-80-3
CMF C14 H16 N4 S

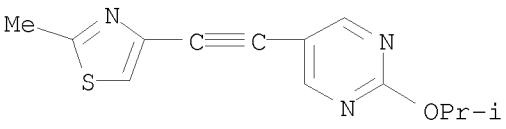


CM 2

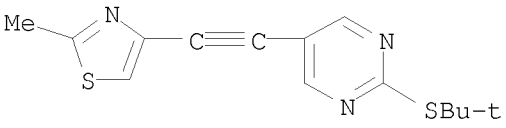
CRN 76-05-1
CMF C2 H F3 O2



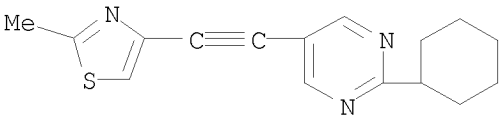
RN 935684-84-7 CAPLUS
CN Pyrimidine, 2-(1-methylethoxy)-5-[2-(2-methyl-4-thiazolyl)ethynyl]- (CA INDEX NAME)



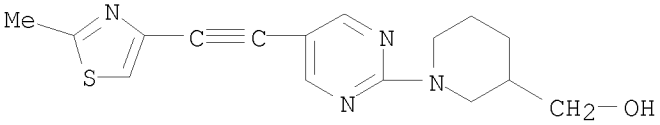
RN 935684-88-1 CAPLUS
CN Pyrimidine, 2-[(1,1-dimethylethyl)thio]-5-[2-(2-methyl-4-thiazolyl)ethynyl]- (CA INDEX NAME)



RN 935684-91-6 CAPLUS
CN Pyrimidine, 2-cyclohexyl-5-[2-(2-methyl-4-thiazolyl)ethynyl]- (CA INDEX NAME)



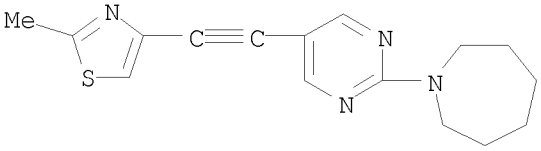
RN 935685-61-3 CAPLUS
CN 3-Piperidinemethanol, 1-[5-[2-(2-methyl-4-thiazolyl)ethynyl]-2-pyrimidinyl]- (CA INDEX NAME)



RN 935685-63-5 CAPLUS
CN 1H-Azepine, hexahydro-1-[5-[2-(2-methyl-4-thiazolyl)ethynyl]-2-pyrimidinyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

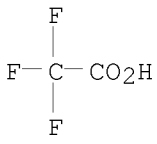
CM 1

CRN 935685-62-4
CMF C16 H18 N4 S



CM 2

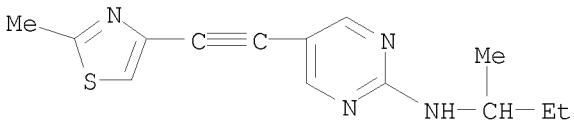
CRN 76-05-1
CMF C2 H F3 O2



RN 935685-65-7 CAPLUS
CN 2-Pyrimidinamine, N-(1-methylpropyl)-5-[2-(2-methyl-4-thiazolyl)ethynyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

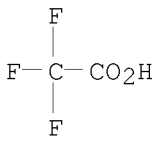
CM 1

CRN 935685-64-6
CMF C14 H16 N4 S



CM 2

CRN 76-05-1
CMF C2 H F3 O2

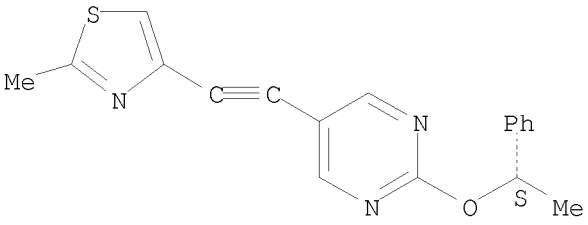


RN 935685-67-9 CAPLUS
CN Pyrimidine, 5-[2-(2-methyl-4-thiazolyl)ethynyl]-2-[(1S)-1-phenylethoxy]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

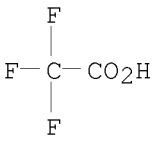
CRN 935685-66-8
CMF C18 H15 N3 O S

Absolute stereochemistry.



CM 2

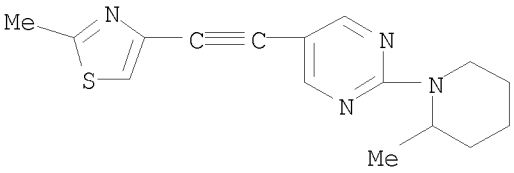
CRN 76-05-1
CMF C2 H F3 O2



RN 935685-69-1 CAPLUS
CN Pyrimidine, 2-(2-methyl-1-piperidinyl)-5-[2-(2-methyl-4-thiazolyl)ethynyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

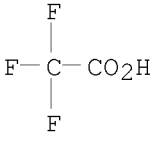
CM 1

CRN 935685-68-0
CMF C16 H18 N4 S



CM 2

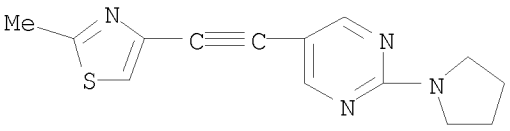
CRN 76-05-1
CMF C2 H F3 O2



RN 935685-71-5 CAPLUS
CN Pyrimidine, 5-[2-(2-methyl-4-thiazolyl)ethynyl]-2-(1-pyrrolidinyl)-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

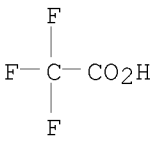
CM 1

CRN 935685-70-4
CMF C14 H14 N4 S

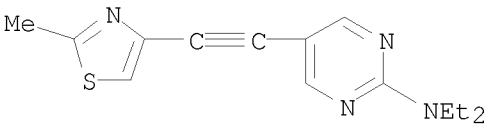


CM 2

CRN 76-05-1
CMF C2 H F3 O2



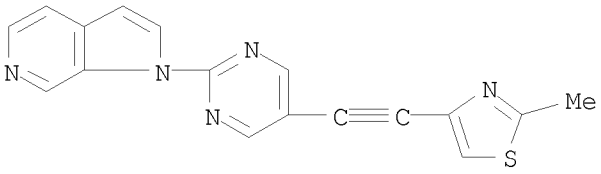
RN 935685-72-6 CAPLUS
CN 2-Pyrimidinamine, N,N-diethyl-5-[2-(2-methyl-4-thiazolyl)ethynyl]- (CA INDEX NAME)



RN 935685-74-8 CAPLUS
CN 1H-Pyrrolo[2,3-c]pyridine, 1-[5-[2-(2-methyl-4-thiazolyl)ethynyl]-2-pyrimidinyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

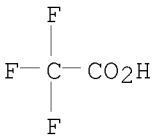
CM 1

CRN 935685-73-7
CMF C17 H11 N5 S



CM 2

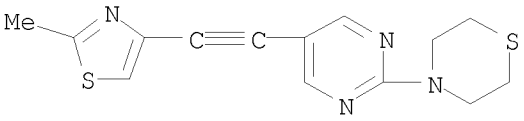
CRN 76-05-1
CMF C2 H F3 O2



RN 935685-76-0 CAPLUS
CN Thiomorpholine, 4-[5-[2-(2-methyl-4-thiazolyl)ethynyl]-2-pyrimidinyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

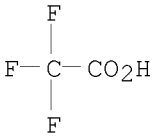
CM 1

CRN 935685-75-9
CMF C14 H14 N4 S2

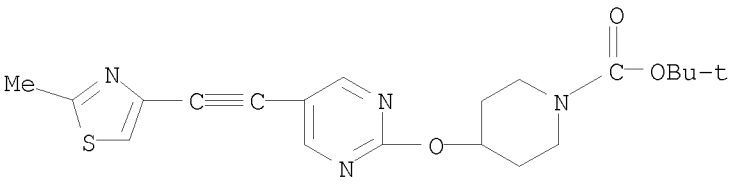


CM 2

CRN 76-05-1
CMF C2 H F3 O2



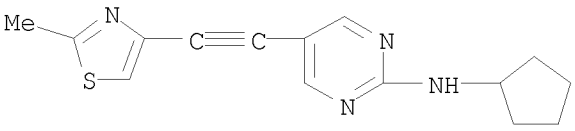
RN 935685-77-1 CAPLUS
CN 1-Piperidinecarboxylic acid, 4-[[5-[2-(2-methyl-4-thiazolyl)ethynyl]-2-pyrimidinyl]oxy]-, 1,1-dimethylethyl ester (CA INDEX NAME)



RN 935685-79-3 CAPLUS
CN 2-Pyrimidinamine, N-cyclopentyl-5-[2-(2-methyl-4-thiazolyl)ethynyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

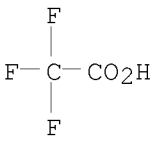
CM 1

CRN 935685-78-2
CMF C15 H16 N4 S



CM 2

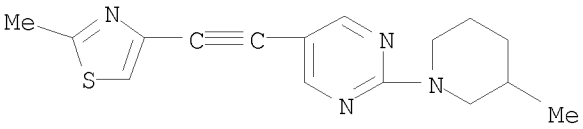
CRN 76-05-1
CMF C2 H F3 O2



RN 935685-81-7 CAPLUS
CN Pyrimidine, 2-(3-methyl-1-piperidinyl)-5-[2-(2-methyl-4-thiazolyl)ethynyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

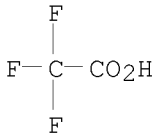
CM 1

CRN 935685-80-6
CMF C16 H18 N4 S



CM 2

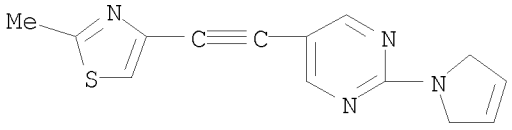
CRN 76-05-1
CMF C2 H F3 O2



RN 935685-83-9 CAPLUS
CN Pyrimidine, 2-(2,5-dihydro-1H-pyrrol-1-yl)-5-[2-(2-methyl-4-thiazolyl)ethynyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

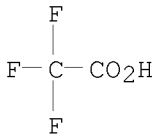
CM 1

CRN 935685-82-8
CMF C14 H12 N4 S



CM 2

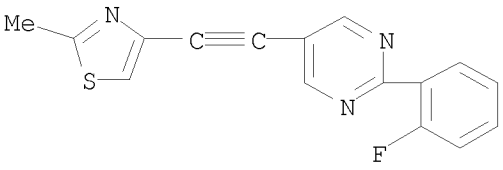
CRN 76-05-1
CMF C2 H F3 O2



RN 935685-85-1 CAPLUS
CN Pyrimidine, 2-(2-fluorophenyl)-5-[2-(2-methyl-4-thiazolyl)ethynyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

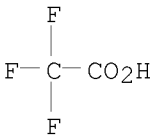
CM 1

CRN 935685-84-0
CMF C16 H10 F N3 S

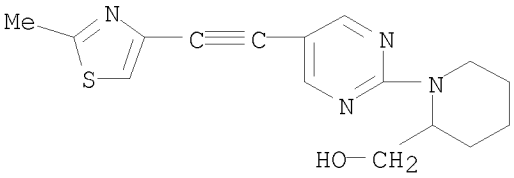


CM 2

CRN 76-05-1
CMF C2 H F3 O2

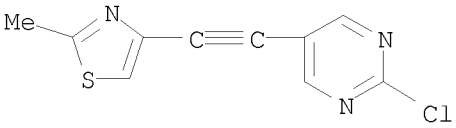


RN 935685-86-2 CAPLUS
CN 2-Piperidinemethanol, 1-[5-[2-(2-methyl-4-thiazolyl)ethynyl]-2-pyrimidinyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

IT 935685-87-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of (thiazolylethynyl)pyridines and -pyrimidines as mGluR5 antagonists)
RN 935685-87-3 CAPLUS
CN Pyrimidine, 2-chloro-5-[2-(2-methyl-4-thiazolyl)ethynyl]- (CA INDEX NAME)



L8 ANSWER 10 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2007:422570 CAPLUS
DN 148:421
TI Bond-based quadratic TOMOCOMD-CARDD molecular indices & statistical techniques for new antitrichomonal drug-like compounds discovery
AU Meneses-Marcel, Alfredo; Rivera-Borroto, Oscar M.; Marrero-Ponce, Yovani; Montero, Alina; Tugores, Yanetsy Machado; Escario, Jose Antonio; Barrio, Alicia Gomez; Pereira, David Montero; Nogal, Juan Jose; Kouznetsov, Vladimir V.; Puentes, Cristian Ochoa; Bohorquez, Arnold R.; Grau, Ricardo; Cancio, Nilo Castanedo; Torrens, Francisco; Ibarra-Velarde, Froylan; Rotondo, Richard; Alvarado, Ysaias J.; Vogel, Christian; Rodriguez-Machin, Lizet
CS Unit of Computer-Aided Molecular "Biosilico" Discovery and Bioinformatics Research, Faculty of Chemistry-Pharmacy and Department of Drug Design, Chemical Bioactive Center, Central University of Las Villas, Villa Clara, 54830, Cuba
SO Proceedings of ECSOC-10, International Electronic Conference on Synthetic Organic Chemistry, 10th, Nov. 1-30, 2006 (2006), c005/1-c005/53. Editor(s): Seijas, Julio A.; Vazquez Tato, M. Pilar. Publisher: Molecular Diversity Preservation International, Basel, Switz. CODEN: 69JDXC; ISBN: 3-906980-18-9
DT Conference; (computer optical disk)
LA English
AB New antitrichomonal agents are needed to combat emerging metronidazole-resistant trichomoniasis and reduce the side-effects associated with currently available drugs. Toward this end, bond-based quadratic indexes, new TOMOCOMD-CARDD mol. descriptors, and linear discriminant anal. (LDA) were used to discover novel, potent, and nontoxic lead trichomonacidal chems. Two discriminant functions were obtained with the use of nonstochastic and stochastic total and bond-type quadratic indexes for heteroatoms. The obtained LDA-based QSAR models, using nonstochastic and stochastic indexes, were able to classify correctly 87.91% (87.50%) and 89.01% (84.38%) of the chems. in training (test) sets, resp. They showed large Matthews' correlation coeffs. (C) of 0.75 (0.71) and 0.78 (0.65) for the training (test) sets, correspondingly. The result of predictions on the 10% full-out cross-validation test also evidenced the robustness of the obtained models. Later, both models were applied to the virtual screening of 12 compds. already proved against Trichomonas Vaginalis (Tv). As a result, they correctly classified 10 out of 12 (83.33%) and 9 out of 12 (75.00%) of the chems., resp.; which is a more important criterion for validating the models. In addition, these classification functions were also applied to a library of twenty-one chems. to find new lead antitrichomonal agents. These compds. were synthesized and tested for in vitro activity against Tv. As expected, theor. results almost coincided with exptl. ones since there was obtained a correct classification for both models of 95.24% (20 out of 21) of the chems. Out of the twenty-one compds. that were screened, and synthesized, two mols. (chems. G-1, UC-245), showed high to moderate cytocidal activity at the concentration of 10 μg/mL, other two compds. (G-0 and CRIS-148) showed high cytocidal activity only at the concentration of 100 μg/mL, and the remaining chems. (from CRIS-105 to CRIS-153 except CRIS-148) were inactive at these assayed concns. Finally, the best candidate, G-1 (cytocidal activity of 100% at 10μg/mL) was in vivo assayed in ovariectomized Wistar rats achieving promissory results as a trichomonacidal drug-like compound The LDA-based QSAR models presented here can be considered as a computer-assisted system that could potentially significantly reduce the number of synthesized and tested compds. and increase the chance of finding

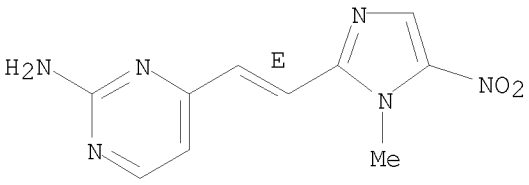
new chemical entities with antitrichomonal activity.

IT 62973-76-6, Azanidazole
RL: PAC (Pharmacological activity); BIOL (Biological study)
(trichomonacide drug discovery)

RN 62973-76-6 CAPLUS

CN 2-Pyrimidinamine, 4-[(1E)-2-(1-methyl-5-nitro-1H-imidazol-2-yl)ethenyl]-
(CA INDEX NAME)

Double bond geometry as shown.

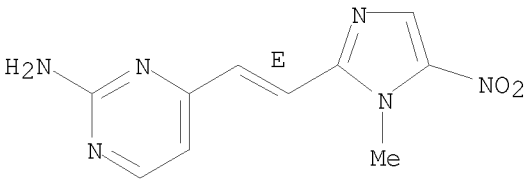


RE.CNT 123 THERE ARE 123 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 11 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2007:422568 CAPLUS
DN 148:420
TI Quick access to potential trichomonacidals through bond linear indices-trained ligand-based virtual screening models
AU Marrero-Ponce, Yovani; Meneses-Marcel, Alfredo; Rivera-Borroto, Oscar M.; Montero, Alina; Escario, Jose Antonio; Barrio, Alicia Gomez; Pereira, David Montero; Nogal, Juan Jose; Grau, Ricardo; Torrens, Francisco; Ibarra-Velarde, Froylan; Rotondo, Richard; Alvarado, Ysaias J.; Vogel, Christian; Rodriguez-Machin, Lizet
CS Unit of Computer-Aided Molecular "Biosilico°s Discovery and Bioinformatic Research, Faculty of Chemistry-Pharmacy and Department of Drug Design, Chemical Bioactive Center, Central University of Las Villas, Villa Clara, 54830, Cuba
SO Proceedings of ECSOC-10, International Electronic Conference on Synthetic Organic Chemistry, 10th, Nov. 1-30, 2006 (2006), c004/1-c004/41. Editor(s): Seijas, Julio A.; Vazquez Tato, M. Pilar. Publisher: Molecular Diversity Preservation International, Basel, Switz. CODEN: 69JDXC; ISBN: 3-906980-18-9
DT Conference; (computer optical disk)
LA English
AB Trichomonas vaginalis (Tv) is the causative agent of the most common, non-viral sexually transmitted disease in women and men worldwide. Since 1959, metronidazole (MTZ) has been the drug of choice in the systemic treatment of trichomoniasis. However, resistance to MTZ in some patients and the great cost associated with the development of new trichomonacidals make necessary the development of computational methods that shorten the drug discovery pipeline. Toward this end, bond-based linear indexes, new TOMOCOMD-CARDD mol. descriptors, and linear discriminant anal. (LDA) were used to discover novel trichomonacidal chems. The models, obtained using non-stochastic and stochastic indexes, were able to classify correctly 89.01% (87.50%) and 82.42% (84.38%) of the chems. in training (test) sets, resp. These results validate the models for use in the ligand-based virtual screening. They also showed large Matthews' correlation coeffs. (C) of 0.78 (0.71) and 0.65 for the training (test) sets, correspondingly. The result of predictions on the 10% full-out cross-validation test also evidenced the robustness of the obtained models. Later, both models were applied to the virtual screening of 12 compds. already proved against Tv. As a result, they correctly classified 10 out of 12 (83.33%) and 9 out of 12 (75.00%) of the chems., resp.; which is a more important criterion for validating the models. In addition, these classification functions were applied to a library of seven chems. to find novel antitrichomonal agents. These compds. were synthesized and tested for in vitro activity against Tv. As a result, exptl. observations approached to theor. predictions since it was obtained a correct classification of 85.71% (6 out of 7) of the chems. Besides, out of the seven compds. that were screened, synthesized and biol. assayed, six compds. (VA7-34, VA7-35, VA7-37, VA7-38, VA7-68, VA7-70) showed pronounced cytocidal activity at the concentration of 100 μg/mL at 24h (48h) within the range of 98.66%-100% (99.40%-100%) while only two mols. (chems. VA7-37 and VA7-38) showed high cytocidal activity at the concentration of 10 μg/mL at 24h (48h): 98.38% (94.23%) and 97.59% (98.10%) correspondingly. The LDA-assisted QSAR models presented here could significantly reduce the number of synthesized and tested compds. and increase the chance of finding new chemical entities with trichomonacidal activity.
IT 62973-76-6, Azanidazole

RL: PAC (Pharmacological activity); BIOL (Biological study)
(QSAR of trichomonacides)
RN 62973-76-6 CAPLUS
CN 2-Pyrimidinamine, 4-[(1E)-2-(1-methyl-5-nitro-1H-imidazol-2-yl)ethenyl]-
(CA INDEX NAME)

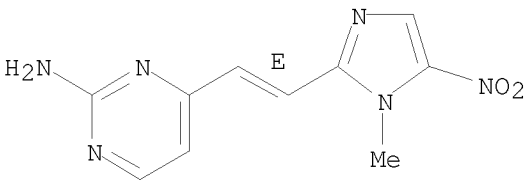
Double bond geometry as shown.



RE.CNT 125 THERE ARE 125 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 12 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2007:366076 CAPLUS
DN 147:22690
TI Quantitative structure vasodilatory activity relationship - synthesis and "in silico" and "in vitro" evaluation of resveratrol-coumarin hybrids
AU Vilar, Santiago; Quezada, Elias; Alcaide, Carlos; Orallo, Francisco; Santana, Lourdes; Uriarte, Eugenio
CS Departamento de Quimica Organica, Facultad de Farmacia, Universidad de Santiago de Compostela, Santiago de Compostela, 15782, Spain
SO QSAR & Combinatorial Science (2007), 26(3), 317-332
CODEN: QCSSAU; ISSN: 1611-020X
PB Wiley-VCH Verlag GmbH & Co. KGaA
DT Journal
LA English
OS CASREACT 147:22690
AB Three theor. models have been developed for the prediction of vasodilatory activity through a series of 2-D mol. descriptors. A database of 501 compds. was selected from the literature and, of these compds., 86 have vasodilatory activity. The QSAR models are capable of differentiating between active and inactive compds. with a level of classification greater than 80%. The models were used to predict the activity of a series of coumarins derived from resveratrol (a natural compound that is present in wine and has good vasodilatory activity) and led to the synthesis of three selected mols. The synthesis of the resveratrol-coumarin hybrids was efficiently achieved through a straight-forward and direct route, and their vasodilatory activities were determined exptl. in rat aorta rings that were pretreated with noradrenaline. The theor. results ("in silico" evaluation) show very good agreement with the exptl. data ("in vitro" evaluation), which provide evidence of the reliability of the theor. calcns. and show their applicability in the rational design of new compds. The compound predicted by the three models to be active (compound 6) was confirmed to be the more active than trans-resveratrol.
IT 62973-76-6, Azanidazole
RL: PAC (Pharmacological activity); PRP (Properties); BIOL (Biological study)
(QSAR vasodilatory activity relationship of resveratrol-coumarin hybrids)
RN 62973-76-6 CAPLUS
CN 2-Pyrimidinamine, 4-[(1E)-2-(1-methyl-5-nitro-1H-imidazol-2-yl)ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.



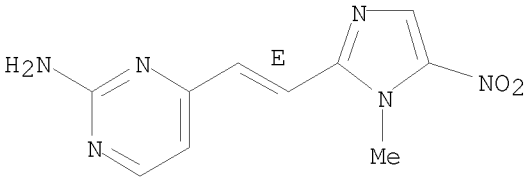
RE.CNT 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 13 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2007:365816 CAPLUS
DN 147:528256
TI Sustained release, mucoadhesive vaginal pharmaceutical compositions
IN Sen, Nilendu; Bhonsle, Shrikant; Prasath, Kaliaperumal Arun; Krishnan, Anandi
PA Glenmark Pharmaceuticals Limited, India
SO Indian Pat. Appl., 39pp.
CODEN: INXXBQ
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI IN 2004MU00555	A	20060505	IN 2004-MU555	20040514
PRAI IN 2004-MU555		20040514		

AB A sustained release mucoadhesive vaginal pharmaceutical composition is provided comprising (a) an effective amount of at least one active pharmaceutical ingredient and (b) a hydrophilic matrix having mucoadhesive properties and capable and capable of providing a sustained release of the active pharmaceutical ingredient, the hydrophilic matrix comprising a water soluble, polyalkylene oxide having a weight average mol. weight of at least about 100,000.
IT 62973-76-6, Azanidazole
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(sustained-release mucoadhesive pharmaceuticals containing hydrophilic matrixes)
RN 62973-76-6 CAPLUS
CN 2-Pyrimidinamine, 4-[(1E)-2-(1-methyl-5-nitro-1H-imidazol-2-yl)ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.



L8 ANSWER 14 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2006:1256641 CAPLUS
DN 146:50262
TI Antibiotic kit and compositions
IN Friedman, Doron; Besonov, Alex; Tamarkin, Dov; Eini, Meir
PA Foamix Ltd., Israel
SO U.S. Pat. Appl. Publ., 31pp., Cont.-in-part of U.S. Ser. No. 532,618.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 26

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 20060269485	A1	20061130	US 2006-448490	20060607
	WO 2004037225	A2	20040506	WO 2003-IB5527	20031024
	WO 2004037225	A3	20041229		
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	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	US 20050069566	A1	20050331	US 2004-911367	20040804
	US 20060140984	A1	20060629	US 2005-532618	20051222
	AU 2006339311	A2	20070907	AU 2006-339311	20060607
	AU 2006339311	A1	20070907		
	CA 2611577	A1	20070907	CA 2006-2611577	20060607
	WO 2007099396	A2	20070907	WO 2006-IB3975	20060607
	WO 2007099396	A3	20080313		
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	RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA				
	EP 1919449	A2	20080514	EP 2006-847249	20060607
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	US 20070292355	A1	20071220	US 2007-732547	20070404
	WO 2008075207	A2	20080626	WO 2007-IB4459	20070404
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TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRAI US 2002-429546P P 20021129
US 2003-492385P P 20030804
WO 2003-IB5527 W 20031024
US 2004-911367 A2 20040804
US 2005-688244P P 20050607
US 2005-532618 A2 20051222
IL 2002-152486 A 20021025
US 2003-497648P P 20030825
US 2003-530015P P 20031216
US 2004-835505 A2 20040428
US 2004-922358 A2 20040820
US 2005-41921 A2 20050124
US 2006-789186P P 20060404
US 2006-448490 A2 20060607
WO 2006-IB3975 W 20060607
US 2006-861620P P 20061129
US 2007-880434P P 20070112

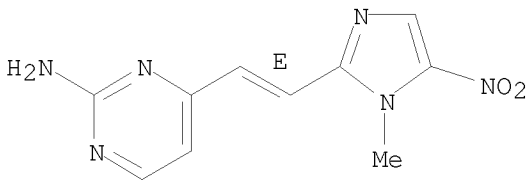
AB The present invention relates to a therapeutic kit to provide an effective dosage of an antibiotic including an aerosol packaging assembly. The assembly includes a container accommodating a pressurized product; and an outlet capable of releasing the pressurized product as a foam, wherein the pressurized product comprises a foamable composition of an antibiotic; at least one organic carrier selected from the group consisting of a hydrophobic organic carrier, an organic polar solvent, an emollient and mixts. at 2-50%, a surfactant, 0.01-5% by weight of at least one polymeric additive selected from the group consisting of a bioadhesive agent, a gelling agent, a film forming agent and a phase change agent, water; and liquefied or compressed gas propellant at 3-25% by weight of the total composition

IT 62973-76-6, Azanidazole
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(antibiotic kit and compns.)

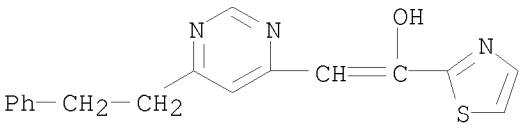
RN 62973-76-6 CAPLUS

CN 2-Pyrimidinamine, 4-[(1E)-2-(1-methyl-5-nitro-1H-imidazol-2-yl)ethenyl]- (CA INDEX NAME)

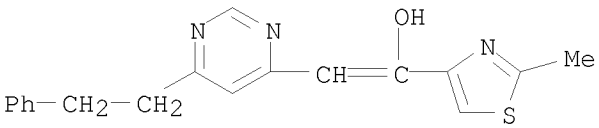
Double bond geometry as shown.



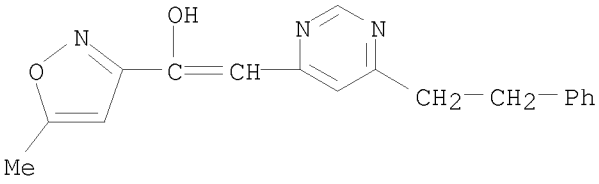
L8 ANSWER 15 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2006:1170544 CAPLUS
DN 146:92611
TI A platform for designing HIV integrase inhibitors. 2-Hydroxy-3-heteroaryl acrylic acid derivatives as novel HIV integrase inhibitor and modeling of hydrophilic and hydrophobic pharmacophores
AU Kawasuji, Takashi; Yoshinaga, Tomokazu; Sato, Akihiko; Yodo, Mitsuaki; Fujiwara, Tamio; Kiyama, Ryuichi
CS Shionogi Research Laboratories, Shionogi & Company, Ltd., Fukushima-ku, Osaka, 553-0002, Japan
SO Bioorganic & Medicinal Chemistry (2006), 14(24), 8430-8445
CODEN: BMECEP; ISSN: 0968-0896
PB Elsevier Ltd.
DT Journal
LA English
OS CASREACT 146:92611
AB The authors present a novel series of HIV integrase inhibitors, showing IC50s ranging from 0.01 to over 370 μM in an enzymic assay. Furthermore, pharmacophore modeling study for the inhibitors was carried out to elucidate the structure-activity relationships. Finally, the authors found a 3D-pharmacophore model, which is composed of a hydrophilic and a hydrophobic domain, providing valuable information for designing other novel types of integrase inhibitors.
IT 329983-05-3P 329983-09-7P 329983-11-1P
329983-12-2P 329983-14-4P
RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(hydroxyheteroaryl acrylic acid derivs. as novel HIV integrase inhibitors and modeling of hydrophilic and hydrophobic pharmacophores)
RN 329983-05-3 CAPLUS
CN 2-Thiazolemethanol, α-[[6-(2-phenylethyl)-4-pyrimidinyl]methylene]- (CA INDEX NAME)



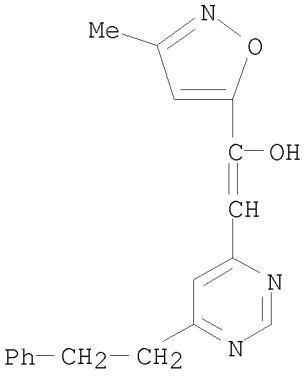
RN 329983-09-7 CAPLUS
CN 4-Thiazolemethanol, 2-methyl-α-[[6-(2-phenylethyl)-4-pyrimidinyl]methylene]- (CA INDEX NAME)



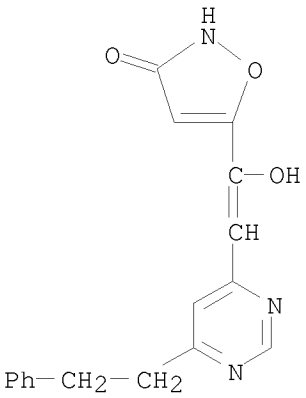
RN 329983-11-1 CAPLUS
CN 3-Isoxazolemethanol, 5-methyl-α-[[6-(2-phenylethyl)-4-pyrimidinyl]methylene]- (CA INDEX NAME)



RN 329983-12-2 CAPLUS
CN 5-Isoxazolemethanol, 3-methyl-α-[[6-(2-phenylethyl)-4-pyrimidinyl]methylene]- (CA INDEX NAME)

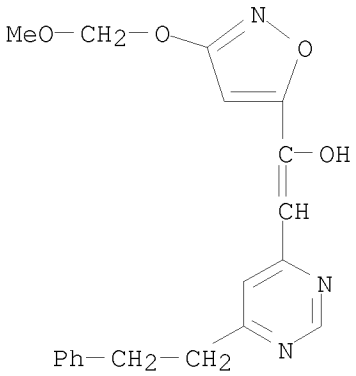


RN 329983-14-4 CAPLUS
CN 3(2H)-Isoxazolone, 5-[1-hydroxy-2-[6-(2-phenylethyl)-4-pyrimidinyl]ethenyl]- (CA INDEX NAME)



IT 329983-06-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(hydroxyheteroaryl acrylic acid derivs. as novel HIV integrase inhibitors and modeling of hydrophilic and hydrophobic pharmacophores)
RN 329983-06-4 CAPLUS
CN 5-Isoxazolemethanol, 3-(methoxymethoxy)-α-[[6-(2-phenylethyl)-4-

pyrimidinyl]methylene]- (CA INDEX NAME)



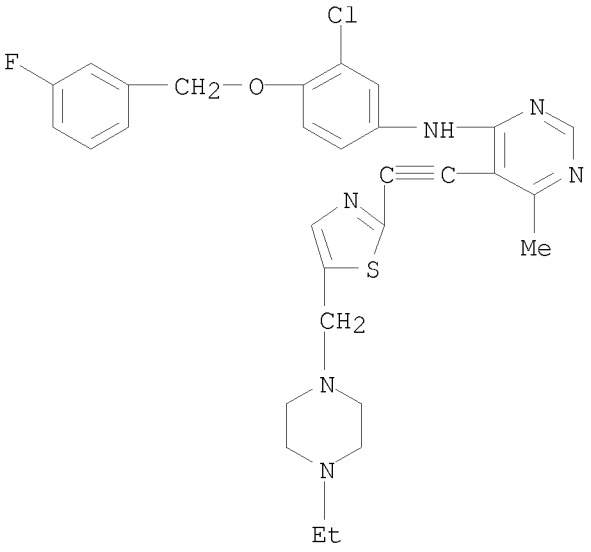
RE.CNT 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 16 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2006:1065980 CAPLUS
DN 145:419166
TI Preparation of pyrimidine derivatives as tyrosine kinase inhibitors
IN Shiota, Takeshi; Suzuki, Naoyuki; Murashi, Takami
PA Shionogi & Co., Ltd., Japan
SO PCT Int. Appl., 117pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

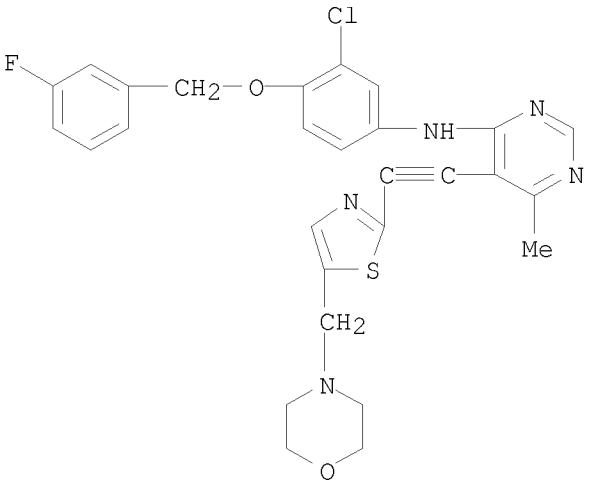
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2006106721	A1	20061012	WO 2006-JP306445	20060329

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRAI JP 2005-97361 A 20050330
OS MARPAT 145:419166
AB Title compds. I [R1 = alkyl, alkyloxy, alkylthio, etc.; R2 = Q1, etc.; R4, R5 = H, (un)substituted alkyl, alkenyl, etc.; R6 = (un)substituted alkyl, alkyloxy, alkoxycarbonyl, etc.; Ar1 = arylene, heteroarylene; R = (un)substituted alkyl, alkyloxy, alkyloxycarbonyl, etc.; n = 0-2; Y = -O-, -S-, -NR20-, etc.; R20 = H, alkyl, acyl, etc.; R3 = Q2, etc.; R22 = H, halo, (un)substituted alkyloxy, etc.; R23, R24 = H, (un)substituted alkyl, (un)substituted alkenyl, etc.], pharmaceutically acceptable salts or solvates thereof were prepared For example, reaction of 4-chloro-5-iodo-6-methylpyrimidine with 3-chloro-4-(3-fluorobenzyloxy)aniline followed by Pd(PPh3)2Cl2 catalyzed coupling with 4-but-3-ynyl-morpholine afforded compound II. In tyrosine kinase inhibition assays, compound II exhibited IC50 values of 19 and 74 nM against EGFR and HER2, resp. Compds. I are claimed useful for the treatment of cancer.
IT 912353-91-4P 912353-95-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrimidine derivs. as tyrosine kinase inhibitors for treatment of cancer)
RN 912353-91-4 CAPLUS
CN 4-Pyrimidinamine, N-[3-chloro-4-[(3-fluorophenyl)methoxy]phenyl]-5-[2-[5-[(4-ethyl-1-piperazinyl)methyl]-2-thiazolyl]ethynyl]-6-methyl- (CA INDEX NAME)



RN 912353-95-8 CAPLUS
CN 4-Pyrimidinamine, N-[3-chloro-4-[(3-fluorophenyl)methoxy]phenyl]-6-methyl-5-[2-[5-(4-morpholinylmethyl)-2-thiazolyl]ethynyl]- (CA INDEX NAME)



RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 17 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2006:1036526 CAPLUS
DN 145:397539
TI Preparation of ethynylpyrimidine derivatives as Tie2 receptor tyrosine kinase inhibitors for the treatment of cancer
IN Jones, Clifford David; Luke, Richard William Arthur; Mccoull, William
PA Astrazeneca AB, Swed.; Astrazeneca Uk Limited
SO PCT Int. Appl., 135pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2006103449	A2	20061005	WO 2006-GB1175	20060330
	WO 2006103449	A3	20070816		
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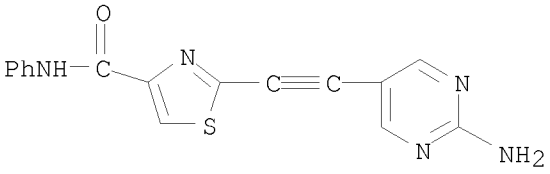
	RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA				
	EP 1893605	A2	20080305	EP 2006-726581	20060330
	R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, MK, YU				
	IN 2007DN07363	A	20071102	IN 2007-DN7363	20070924
	CN 101198602	A	20080611	CN 2006-80019050	20071129
PRAI	GB 2005-6467	A	20050331		
	GB 2005-12611	A	20050621		
	GB 2005-12615	A	20050621		
	WO 2006-GB1175	W	20060330		

OS MARPAT 145:397539
AB Title compds. I [one of Ra and Rb is NR1R2, and the other is R3 or R4; Rc = R3 or R4; R1, R2 = H, alkylsulfonyl, Ph, etc.; R1 and R2 may link together to form a ring; R3, R4 = NR1R2, H, (un)substituted alkyl, etc.; ring A = (hetero)aryl; R5 = cyclopropyl, cyano, halo, etc.; n = 0-3; L = (un)substituted amide, (un)substituted amine, alkyl group, etc.; ring B = cycloalkyl, heterocyclyl,(hetero)aryl,etc.; R6 = alkyl, alkoxy, alkylsulfonyl, etc.; m = 0-3, with limitations] or salts and solvates thereof were prepared as Tie2 receptor tyrosine kinase inhibitors. For instance, PdCl2dppf/CuI-catalyzed coupling of 2-amino-5-iodopyrimidine with trimethylsilylacetylene (100%) followed by desilylation under acidic condition (100%) gave 5-ethynylpyrimidin-2-amine (II). Successive amidation of 5-bromothiophene-2-carbonyl chloride with 2-fluoro-5-(trifluoromethyl)aniline (27%), and coupling of the resultant bromide with acetylene II catalyzed by (PPh3)4Pd/CuI (52%) led to ethynylpyrimidinamine III. I generally showed inhibition of autophosphorylation of Tie2 receptor tyrosine kinase with IC50 values of < 50 μM in a cellular assay. Therefore, I and their pharmaceutical compns. are useful for the treatment of cancer in warm-blooded animals and

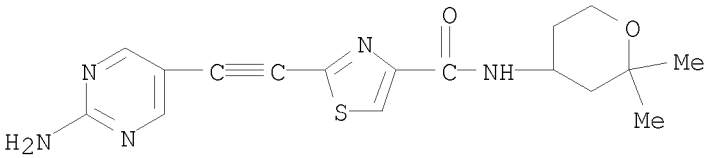
in the production of medicaments with anti-angiogenic effect. The invention also relates to processes for the preparation of I.

IT 911433-65-3P 911433-68-6P 911433-69-7P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of ethynylpyrimidine derivs. as Tie2 receptor tyrosine kinase inhibitors for the treatment of cancer)

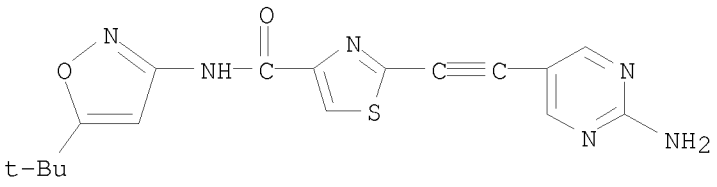
RN 911433-65-3 CAPLUS
CN 4-Thiazolecarboxamide, 2-[2-(2-amino-5-pyrimidinyl)ethynyl]-N-phenyl- (CA INDEX NAME)



RN 911433-68-6 CAPLUS
CN 4-Thiazolecarboxamide, 2-[2-(2-amino-5-pyrimidinyl)ethynyl]-N-(tetrahydro-2,2-dimethyl-2H-pyran-4-yl)- (CA INDEX NAME)

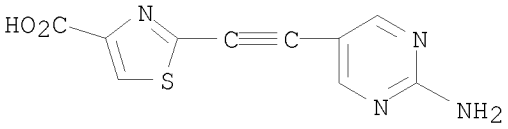


RN 911433-69-7 CAPLUS
CN 4-Thiazolecarboxamide, 2-[2-(2-amino-5-pyrimidinyl)ethynyl]-N-[5-(1,1-dimethylethyl)-3-isoxazolyl]- (CA INDEX NAME)

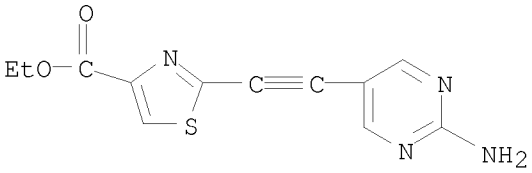


IT 911433-66-4P 911433-67-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of ethynylpyrimidine derivs. as Tie2 receptor tyrosine kinase inhibitors for the treatment of cancer)

RN 911433-66-4 CAPLUS
CN 4-Thiazolecarboxylic acid, 2-[2-(2-amino-5-pyrimidinyl)ethynyl]- (CA INDEX NAME)



RN 911433-67-5 CAPLUS
CN 4-Thiazolecarboxylic acid, 2-[2-(2-amino-5-pyrimidinyl)ethynyl]-, ethyl ester (CA INDEX NAME)



L8 ANSWER 18 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2006:1011718 CAPLUS
DN 145:377377
TI Preparation of acetylenyl-pyrazolo-pyrimidine derivatives for use as mglur2 antagonists treating CNS disorders
IN Gatti McArthur, Silvia; Goetschi, Erwin; Palmer, Wylie Solang; Wichmann, Juergen; Woltering, Thomas Johannes
PA F. Hoffmann-La Roche A.-G., Switz.
SO PCT Int. Appl., 229pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

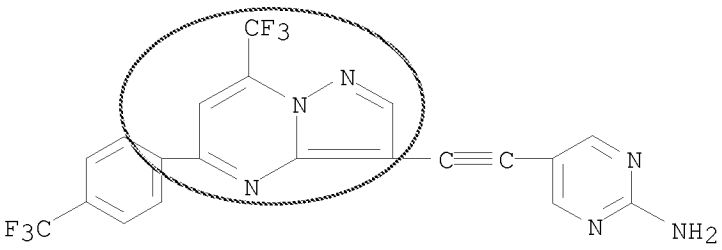
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2006099972	A1	20060928	WO 2006-EP2334	20060314
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	AU 2006226669	A1	20060928	AU 2006-226669	20060314
	CA 2602444	A1	20060928	CA 2006-2602444	20060314
	EP 1863818	A1	20071212	EP 2006-723412	20060314
	R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR				
	US 20060217387	A1	20060928	US 2006-375834	20060315
	US 7238808	B2	20070703		
	US 20070167460	A1	20070719	US 2007-726807	20070323
	NO 2007004592	A	20071019	NO 2007-4592	20070911
	MX 200711483	A	20071012	MX 2007-11483	20070918
	IN 2007CN04169	A	20071116	IN 2007-CN4169	20070924
	KR 2007122221	A	20071228	KR 2007-724199	20071022
	CN 101180299	A	20080514	CN 2006-80018120	20071123
PRAI	EP 2005-102332	A	20050323		
	WO 2006-EP2334	W	20060314		
	US 2006-375834	A3	20060315		

OS MARPAT 145:377377
AB Acetylenyl-pyrazolo-pyrimidine derivs. I, wherein E and J are N, G is C and one of L or M is N and the other is CH; or L and G are N, E is C, and J and M are CH; or J, G and L are N, E is C and M is CH; or E and L are N, J and M are CH and G i s C; R1 is H, halo, CF3, CHF2 or alkyl; R2 is H, halo, alkyl, etc.; R3 is H, alkyl, cycloalkyl; A is an aryl or (un)substituted 5- or 6-membered heteroaryl ring are prepared and useful in the treatment of CNS disorders. Thus, II was prepared and tested as a group II mGlu receptor antagonist with a Ki of 0.001 μM. Further, I can be employed in the treatment of diseases related to mGluR2 activation such as psychosis, schizophrenia, Alzheimer's disease, cognitive disorders, memory deficits or glioma.
IT 911117-96-9P 911118-73-5P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of acetylenyl-pyrazolo-pyrimidine derivs. for use as mglur2 antagonists treating CNS disorders)

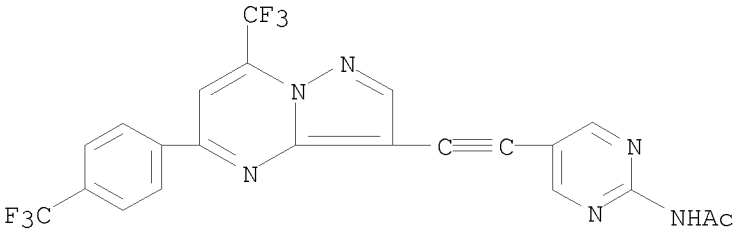
RN 911117-96-9 CAPLUS

CN 2-Pyrimidinamine, 5-[2-[7-(trifluoromethyl)-5-[4-(trifluoromethyl)phenyl]pyrazolo[1,5-a]pyrimidin-3-yl]ethynyl]- (CA INDEX NAME)



RN 911118-73-5 CAPLUS

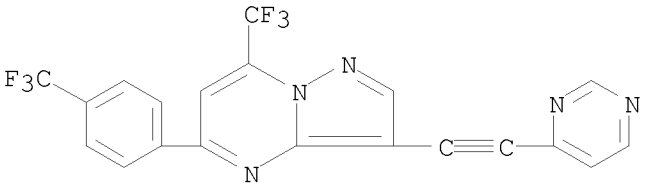
CN Acetamide, N-[5-[2-[7-(trifluoromethyl)-5-[4-(trifluoromethyl)phenyl]pyrazolo[1,5-a]pyrimidin-3-yl]ethynyl]-2-pyrimidinyl]- (CA INDEX NAME)



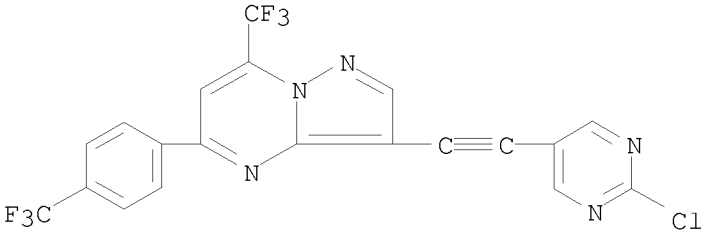
IT 911114-97-1P 911117-48-1P 911117-50-5P
911118-11-1P 911118-24-6P 911118-26-8P
911118-38-2P 911118-61-1P 911118-65-5P
911118-69-9P 911118-71-3P 911119-55-6P
911120-17-7P 911120-19-9P 911120-21-3P
911120-23-5P 911120-25-7P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of acetylenyl-pyrazolo-pyrimidine derivs. for use as mglur2 antagonists treating CNS disorders)

RN 911114-97-1 CAPLUS

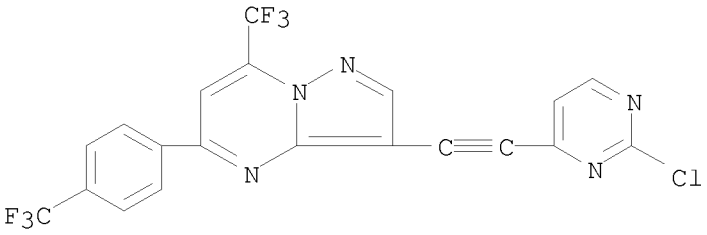
CN Pyrazolo[1,5-a]pyrimidine, 3-[2-(4-pyrimidinyl)ethynyl]-7-(trifluoromethyl)-5-[4-(trifluoromethyl)phenyl]- (CA INDEX NAME)



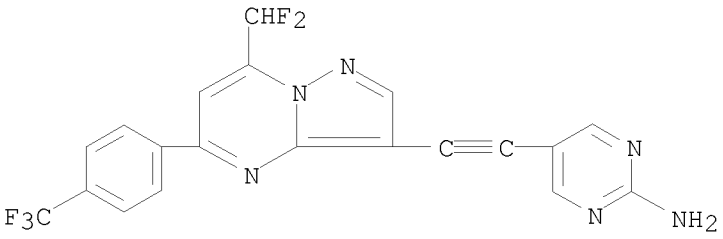
RN 911117-48-1 CAPLUS
CN Pyrazolo[1,5-a]pyrimidine, 3-[2-(2-chloro-5-pyrimidinyl)ethynyl]-7-(trifluoromethyl)-5-[4-(trifluoromethyl)phenyl]- (CA INDEX NAME)



RN 911117-50-5 CAPLUS
CN Pyrazolo[1,5-a]pyrimidine, 3-[2-(2-chloro-4-pyrimidinyl)ethynyl]-7-(trifluoromethyl)-5-[4-(trifluoromethyl)phenyl]- (CA INDEX NAME)

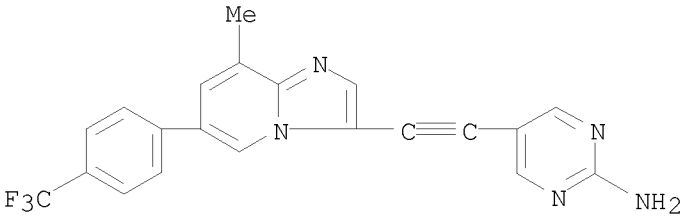


RN 911118-11-1 CAPLUS
CN 2-Pyrimidinamine, 5-[2-[7-(difluoromethyl)-5-[4-(trifluoromethyl)phenyl]pyrazolo[1,5-a]pyrimidin-3-yl]ethynyl]- (CA INDEX NAME)

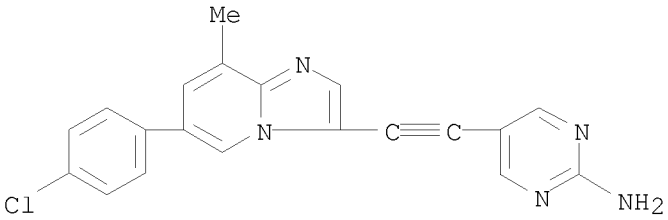


RN 911118-24-6 CAPLUS

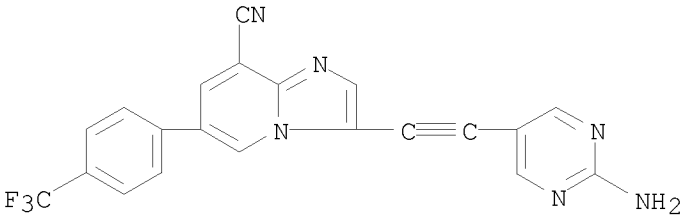
CN 2-Pyrimidinamine, 5-[2-[8-methyl-6-[4-(trifluoromethyl)phenyl]imidazo[1,2-a]pyridin-3-yl]ethynyl]- (CA INDEX NAME)



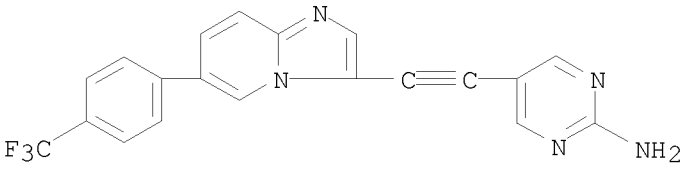
RN 911118-26-8 CAPLUS
CN 2-Pyrimidinamine, 5-[2-[6-(4-chlorophenyl)-8-methylimidazo[1,2-a]pyridin-3-yl]ethynyl]- (CA INDEX NAME)



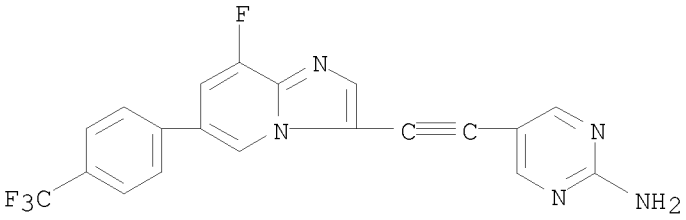
RN 911118-38-2 CAPLUS
CN Imidazo[1,2-a]pyridine-8-carbonitrile, 3-[2-(2-amino-5-pyrimidinyl)ethynyl]-6-[4-(trifluoromethyl)phenyl]- (CA INDEX NAME)



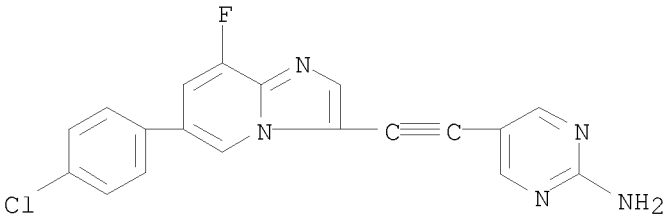
RN 911118-61-1 CAPLUS
CN 2-Pyrimidinamine, 5-[2-[6-[4-(trifluoromethyl)phenyl]imidazo[1,2-a]pyridin-3-yl]ethynyl]- (CA INDEX NAME)



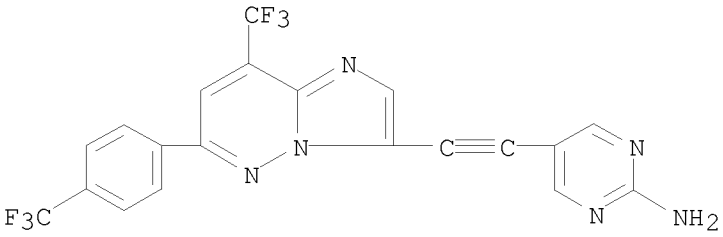
RN 911118-65-5 CAPLUS
CN 2-Pyrimidinamine, 5-[2-[8-fluoro-6-[4-(trifluoromethyl)phenyl]imidazo[1,2-a]pyridin-3-yl]ethynyl]- (CA INDEX NAME)



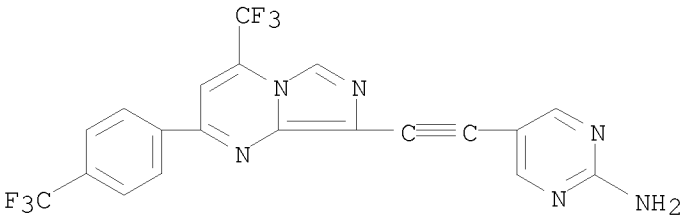
RN 911118-69-9 CAPLUS
CN 2-Pyrimidinamine, 5-[2-[6-(4-chlorophenyl)-8-fluoroimidazo[1,2-a]pyridin-3-yl]ethynyl]- (CA INDEX NAME)



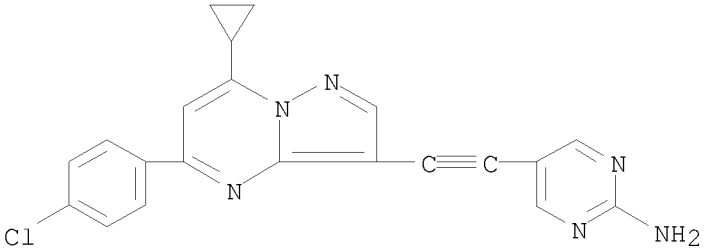
RN 911118-71-3 CAPLUS
CN 2-Pyrimidinamine, 5-[2-[8-(trifluoromethyl)-6-[4-(trifluoromethyl)phenyl]imidazo[1,2-b]pyridazin-3-yl]ethynyl]- (CA INDEX NAME)



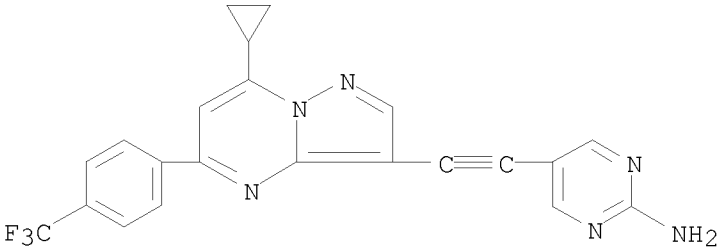
RN 911119-55-6 CAPLUS
CN 2-Pyrimidinamine, 5-[2-[4-(trifluoromethyl)-2-[4-(trifluoromethyl)phenyl]imidazo[1,5-a]pyrimidin-8-yl]ethynyl]- (CA INDEX NAME)



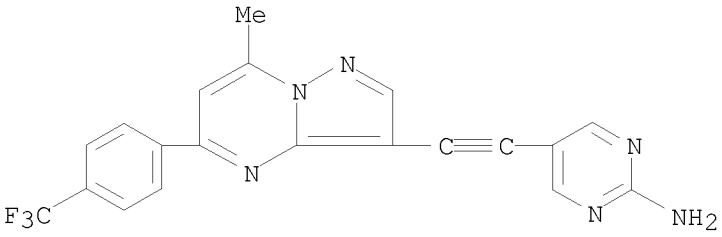
RN 911120-17-7 CAPLUS
CN 2-Pyrimidinamine, 5-[2-[5-(4-chlorophenyl)-7-cyclopropylpyrazolo[1,5-a]pyrimidin-3-yl]ethynyl]- (CA INDEX NAME)



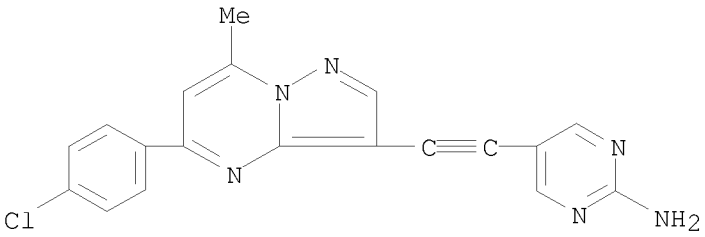
RN 911120-19-9 CAPLUS
CN 2-Pyrimidinamine, 5-[2-[7-cyclopropyl-5-[4-(trifluoromethyl)phenyl]pyrazolo[1,5-a]pyrimidin-3-yl]ethynyl]- (CA INDEX NAME)



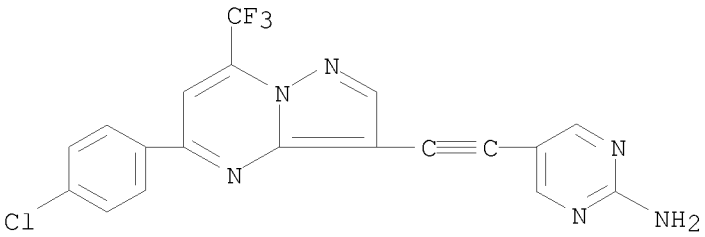
RN 911120-21-3 CAPLUS
CN 2-Pyrimidinamine, 5-[2-[7-methyl-5-[4-(trifluoromethyl)phenyl]pyrazolo[1,5-a]pyrimidin-3-yl]ethynyl]- (CA INDEX NAME)



RN 911120-23-5 CAPLUS
CN 2-Pyrimidinamine, 5-[2-[5-(4-chlorophenyl)-7-methylpyrazolo[1,5-a]pyrimidin-3-yl]ethynyl]- (CA INDEX NAME)



RN 911120-25-7 CAPLUS
CN 2-Pyrimidinamine, 5-[2-[5-(4-chlorophenyl)-7-(trifluoromethyl)pyrazolo[1,5-a]pyrimidin-3-yl]ethynyl]- (CA INDEX NAME)



RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 19 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2006:847169 CAPLUS
DN 145:410015
TI Predicting antitrichomonal activity: A computational screening using atom-based bilinear indices and experimental proofs
AU Marrero-Ponce, Yovani; Meneses-Marcel, Alfredo; Castillo-Garit, Juan A.; Machado-Tugores, Yanetsy; Escario, Jose Antonio; Barrio, Alicia Gomez; Pereira, David Montero; Nogal-Ruiz, Juan Jose; Aran, Vicente J.; Martinez-Fernandez, Antonio R.; Torrens, Francisco; Rotondo, Richard; Ibarra-Velarde, Froylan; Alvarado, Ysaias J.
CS Institut Universitari de Ciencia Molecular, Universitat de Valencia, Edifici d'Instituts de Paterna, Valencia, E-46071, Spain
SO Bioorganic & Medicinal Chemistry (2006), 14(19), 6502-6524
CODEN: BMECEP; ISSN: 0968-0896
PB Elsevier Ltd.
DT Journal
LA English
AB Existing Trichomonas vaginalis therapies are out of reach for most trichomoniasis people in developing countries and, where available, they are limited by their toxicity (mainly in pregnant women) and their cost. New antitrichomonal agents are needed to combat emerging metronidazole-resistant trichomoniasis and reduce the side effects associated with currently available drugs. Toward this end, atom-based bilinear indexes, a new TOMOCOMD-CARDD mol. descriptor, and linear discriminant anal. (LDA) were used to discover novel, potent, and nontoxic lead trichomonacidal chems. Two discriminant functions were obtained with the use of nonstochastic and stochastic atom-type bilinear indexes for heteroatoms and H-bonding of heteroatoms. These atomic-level mol. descriptors were calculated using a weighting scheme that includes four atomic labels, namely atomic masses, van der Waals vols., atomic polarizabilities, and atomic electronegativities in Pauling scale. The obtained LDA-based QSAR models, using nonstochastic and stochastic indexes, were able to classify correctly 94.51% (90.63%) and 93.41% (93.75%) of the chems. in training (test) sets, resp. They showed large Matthews' correlation coeffs. (C); 0.89 (0.79) and 0.87 (0.85), for the training (test) sets, correspondingly. The result of predictions on the 15% full-out cross-validation test also evidenced the robustness and predictive power of the obtained models. In addition, canonical regression analyses corroborated the statistical quality of these models (Rcan of 0.749 and of 0.845, correspondingly); they were also used to compute biol. activity canonical scores for each compound On the other hand, a close inspection of the mol. descriptors included in both equations showed that several of these mol. fingerprints are strongly interrelated with each other. Therefore, these models were orthogonalized using the Randic orthogonalization procedure. These classification functions were then applied to find new lead antitrichomonal agents and six compds. were selected as possible active compds. by computational screening. The designed compds. were synthesized and tested for in vitro activity against T. vaginalis. Out of the six compds. that were designed, and synthesized, three mols. showed high to moderate cytocidal activity at the concentration of 10 μg/mL, other two compds. showed high cytocidal and cytostatic activity at the concentration of 100 μg/mL and 10 μg/mL, correspondingly, and the remaining chemical was inactive at these assayed concns. Nonetheless, these compds. possess structural features not seen in known trichomonacidal compds. and thus can serve as excellent leads for further optimization of antitrichomonal activity. The LDA-based QSAR models presented here can be

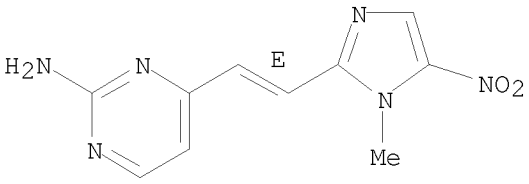
considered as a computer-assisted system that could potentially significantly reduce the number of synthesized and tested compds. and increase the chance of finding new chemical entities with antitrichomonal activity.

IT 62973-76-6, Azanidazole
RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(predicting antitrichomonal activity through a computational screening using atom-based bilinear indexes and exptl. proofs)

RN 62973-76-6 CAPLUS

CN 2-Pyrimidinamine, 4-[(1E)-2-(1-methyl-5-nitro-1H-imidazol-2-yl)ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.



RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 20 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2006:790854 CAPLUS
DN 145:230644
TI Preparation of pyrimidine derivatives and their use as Tie2 receptor tyrosine kinase inhibitors
IN Jones, Clifford David; Luke, Richard William Arthur; Mccoull, William
PA Astrazeneca AB, Swed.; Astrazeneca Uk Limited
SO PCT Int. Appl., 168pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

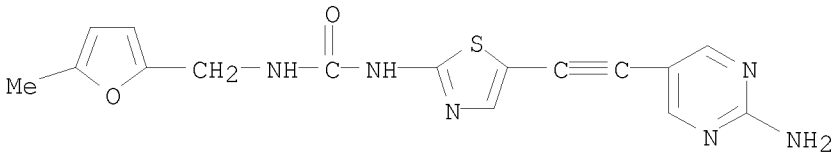
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2006082373	A1	20060810	WO 2006-GB284	20060127
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	EP 1863805	A1	20071212	EP 2006-701245	20060127
	R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR				
	IN 2007DN05604	A	20070817	IN 2007-DN5604	20070719
	CN 101137652	A	20080305	CN 2006-80007855	20070911
PRAI	GB 2005-1984	A	20050201		
	GB 2005-2417	A	20050205		
	GB 2005-12614	A	20050621		
	WO 2006-GB284	W	20060127		

OS MARPAT 145:230644
AB Substituted pyrimidine derivs. I, wherein R1 is an (un)substituted amine, (un)substituted 3-7 membered heterocyclic ring; R2 and R3 are H, (un)substituted alkyl, (un)substituted alkoxy; A is a 5 or 6 membered heteroaryl ring; R4 is halo, cyano, alkoxy, cyclopropyl, alkyl, where the alkoxy or alkyl groups are optionally substituted by cyano or 1 or more fluoro groups; L is meta or para attached by an (un)substituted amide, (un)substituted amine, alkyl group; B is a cycloalkyl, heterocyclic ring, aryl, heteroaryl, bicyclic ring; R5 is a halo, hydroxyl, amino, alkylamino, cyano, cycloalkyl ring, an (un)substituted 3 to 7 membered heterocyclic ring; m and n are 0-3 are prepared and used as as medicaments and in the production of an anti-angiogenic effect in a warm blooded animal. Thus, II was prepared and tested as an in vitro inhibitor of the Tie2 receptor tyrosine kinase and in the inhibition of autophosphorylation of Tie2 receptor tyrosine kinase (IC50 are 1.5 and 1.9 μM resp.). Further, I can be used in the treatment of cancer and as antineoplastic prodrugs.
IT 905439-18-1P 905439-20-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of pyrimidine derivs. and their use as Tie2 receptor tyrosine kinase inhibitors)

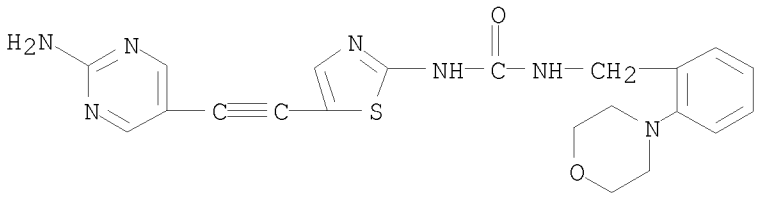
RN 905439-18-1 CAPLUS

CN Urea, N-[5-[2-(2-amino-5-pyrimidinyl)ethynyl]-2-thiazolyl]-N'-[(5-methyl-2-furanyl)methyl]- (CA INDEX NAME)



RN 905439-20-5 CAPLUS

CN Urea, N-[5-[2-(2-amino-5-pyrimidinyl)ethynyl]-2-thiazolyl]-N'-[[2-(4-morpholinyl)phenyl]methyl]- (CA INDEX NAME)

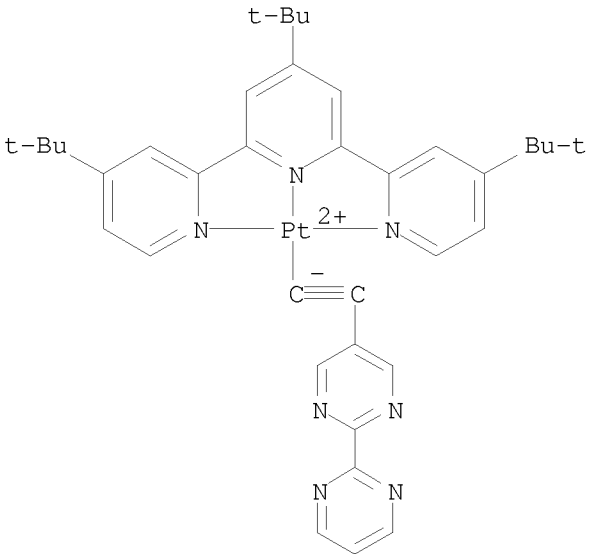


RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 21 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2006:548728 CAPLUS
DN 145:211149
TI Step-controlled synthesis of platinum(II) acetylide frameworks from conjugated polyaromatic modules
AU Ziessel, Raymond; Diring, Stephane
CS Laboratoire de Chimie Moleculaire, Ecole de Chimie, Polymeres, Materiaux (ECPM), Universite Louis Pasteur (ULP), Strasbourg, 67087, Fr.
SO Tetrahedron Letters (2006), 47(27), 4687-4692
CODEN: TELEAY; ISSN: 0040-4039
PB Elsevier B.V.
DT Journal
LA English
OS CASREACT 145:211149
AB A simple synthetic route for the efficient preparation of mono- and dinuclear platinum(II) derivs. containing σ-bonded ethynyl aryl groups is described. A dinuclear complex pointing its two Pt-Cl dipoles in opposite directions is prepared either by complexation of a back-to-back terpyridine ligand with platinum salts or by cross-coupling [(4'-ethynylterpyridine)PtCl] with dibromodidodecylphenyl derivs. FT-IR, UV-vis absorption and cyclic voltammetry are used as spectroscopic tools to characterize these new complexes.
IT 903908-20-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(step-controlled preparation and characterization of platinum acetylide frameworks from conjugated polyarom. modules)
RN 903908-20-3 CAPLUS
CN Platinum(1+), ([2,2'-bipyrimidin]-5-ylethynyl)[4,4',4''-tris(1,1-dimethylethyl)-2,2':6',2''-terpyridine-κN1,κN1',κN1'']-, (SP-4-3)-, tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

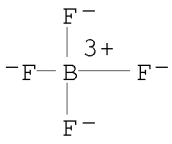
CM 1

CRN 903908-19-0
CMF C37 H40 N7 Pt
CCI CCS



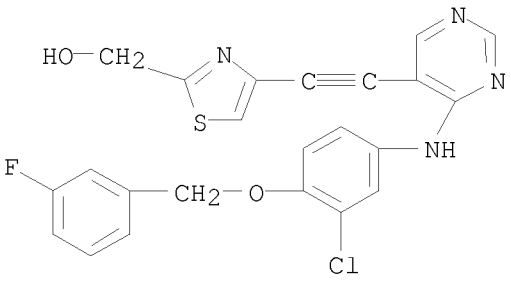
CM 2

CRN 14874-70-5
CMF B F4
CCI CCS

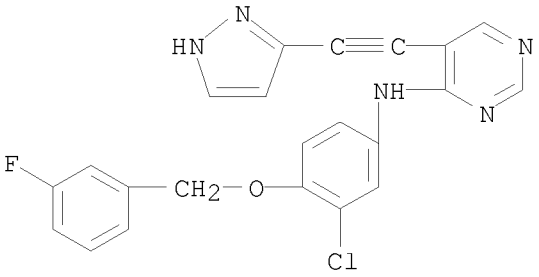


RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 22 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2006:274296 CAPLUS
DN 144:488615
TI Alkynyl pyrimidines as dual EGFR/ErbB2 kinase inhibitors
AU Waterson, Alex G.; Stevens, Kirk L.; Reno, Michael J.; Zhang, Yue-Mei; Boros, Eric E.; Bouvier, Frederic; Rastagar, Abdullah; Uehling, David E.; Dickerson, Scott H.; Reep, Bryan; McDonald, Octerloney B.; Wood, Edgar R.; Rusnak, David W.; Alligood, Krystal J.; Rudolph, Sharon K.
CS GlaxoSmithKline, Research Triangle Park, NC, 27709-3398, USA
SO Bioorganic & Medicinal Chemistry Letters (2006), 16(9), 2419-2422
CODEN: BMCLE8; ISSN: 0960-894X
PB Elsevier B.V.
DT Journal
LA English
OS CASREACT 144:488615
AB Anilinoalkynylpyrimidines were prepared and evaluated as dual EGFR/ErbB2 kinase inhibitors. A preference was found for substituted Ph and heteroarom. rings attached to the alkyne. In addition, the presence of a potential hydrogen bond donor appended to this ring was favored. Selected mols. in the series demonstrated some activity against human tumor cell lines.
IT 845657-58-1P 887147-52-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of alkynyl pyrimidines as dual EGFR/ErbB2 kinase inhibitors)
RN 845657-58-1 CAPLUS
CN 2-Thiazolemethanol, 4-[2-[4-[[3-chloro-4-[(3-fluorophenyl)methoxy]phenyl]amino]-5-pyrimidinyl]ethynyl]- (CA INDEX NAME)



RN 887147-52-6 CAPLUS
CN 4-Pyrimidinamine, N-[3-chloro-4-[(3-fluorophenyl)methoxy]phenyl]-5-[2-(1H-pyrazol-3-yl)ethynyl]- (CA INDEX NAME)



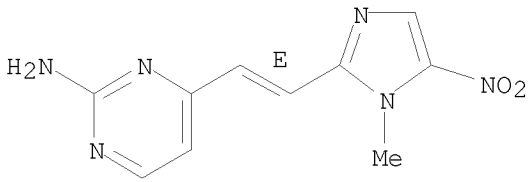
RE.CNT 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 23 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2006:100738 CAPLUS
DN 144:198849
TI Novel dosage form comprising modified-release and immediate-release active ingredients
IN Vaya, Navin; Karan, Rajesh Singh; Sadanand, Sunil; Gupta, Vinod Kumar
PA India
SO U.S. Pat. Appl. Publ., 49 pp., Cont.-in-part of U.S. Ser. No. 630,446.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 2

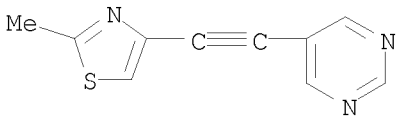
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 20060024365	A1	20060202	US 2005-134633	20050519
	IN 2002MU00697	A	20040529	IN 2002-MU697	20020805
	IN 193042	A1	20040626		
	IN 2002MU00699	A	20040529	IN 2002-MU699	20020805
	IN 2003MU00080	A	20050204	IN 2003-MU80	20030122
	IN 2003MU00082	A	20050204	IN 2003-MU82	20030122
	US 20040096499	A1	20040520	US 2003-630446	20030729
PRAI	IN 2002-MU697	A	20020805		
	IN 2002-MU699	A	20020805		
	IN 2003-MU80	A	20030122		
	IN 2003-MU82	A	20030122		
	US 2003-630446	A2	20030729		

AB A dosage form comprising of a high dose, high solubility active ingredient as modified release and a low dose active ingredient as immediate release where the weight ratio of immediate release active ingredient and modified release active ingredient is from 1:10 to 1:15000 and the weight of modified release active ingredient per unit is from 500 mg to 1500 mg; a process for preparing the dosage form. Tablets containing 10 mg sodium pravastatin and 1000 mg niacin were prepared The release of sodium pravastatin after 24 h was 67.7%, and the release of niacin after 1 h was 84.1%.
IT 62973-76-6, Azanidazole
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(novel dosage form comprising modified-release and immediate-release active ingredients)
RN 62973-76-6 CAPLUS
CN 2-Pyrimidinamine, 4-[(1E)-2-(1-methyl-5-nitro-1H-imidazol-2-yl)ethenyl]-
(CA INDEX NAME)

Double bond geometry as shown.



L8 ANSWER 24 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2006:20956 CAPLUS
DN 144:274179
TI Synthesis and Structure-Activity Relationships of 3-[(2-Methyl-1,3-thiazol-4-yl)ethynyl]pyridine Analogues as Potent, Noncompetitive Metabotropic Glutamate Receptor Subtype 5 Antagonists; Search for Cocaine Medications
AU Iso, Yasuyoshi; Grajkowska, Ewa; Wroblewski, Jarda T.; Davis, Jared; Goeders, Nicholas E.; Johnson, Kenneth M.; Sanker, Subramaniam; Roth, Bryan L.; Tueckmantel, Werner; Kozikowski, Alan P.
CS Drug Discovery Program, Department of Medicinal Chemistry and Pharmacognosy, University of Illinois at Chicago, Chicago, IL, 60612, USA
SO Journal of Medicinal Chemistry (2006), 49(3), 1080-1100
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
OS CASREACT 144:274179
AB Recent genetic and pharmacol. studies have suggested that the metabotropic glutamate receptor subtype 5 (mGluR5) may represent a druggable target in identifying new therapeutics for the treatment of various central nervous system disorders including drug abuse. In particular, considerable attention in the mGluR5 field has been devoted to identifying ligands that bind to the allosteric modulatory site, distinct from the site for the primary agonist glutamate. Both 2-methyl-6-(phenylethynyl)pyridine (MPEP) and its analog 3-[(2-methyl-4-thiazolyl)ethynyl]pyridine (MTEP) have been shown to be selective and potent noncompetitive antagonists of mGluR5. Because of results presented in this study showing that MTEP prevents the reinstatement of cocaine self-administration caused by the presentation of environmental cues previously associated with cocaine availability, a series of analogs of MTEP was prepared with the aim of gaining a better understanding of the structural features relevant to its antagonist potency and with the ultimate aim of investigating the effects of such compds. in blunting the self-administration of cocaine. These efforts have led to the identification of compds. showing higher potency as mGluR5 antagonists than either MPEP or MTEP. Two compds. exhibited functional activity as mGluR5 antagonists that are 490 and 230 times, resp., better than that of MTEP.
IT 329205-90-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of methyl[(pyrimidinyl)ethynyl]thiazole derivs. and study of their activity as noncompetitive metabotropic glutamate receptor subtype-5 (mGluR5) antagonists)
RN 329205-90-5 CAPLUS
CN Pyrimidine, 5-[2-(2-methyl-4-thiazolyl)ethynyl]- (CA INDEX NAME)



RE.CNT 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 25 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2005:1224669 CAPLUS
DN 143:466245
TI Sustained-release mucoadhesive vaginal pharmaceutical compositions
IN Sen, Nilendu; Prasath, Kaliaperumal Arun; Bhonsle, Shrikant; Krishnan, Anandi
PA Glenmark Pharmaceuticals Limited, India
SO PCT Int. Appl., 25 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

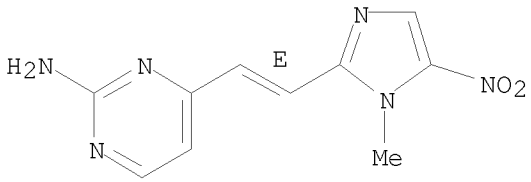
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2005107702	A2	20051117	WO 2005-IB1277	20050511
WO 2005107702	A3	20061005		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

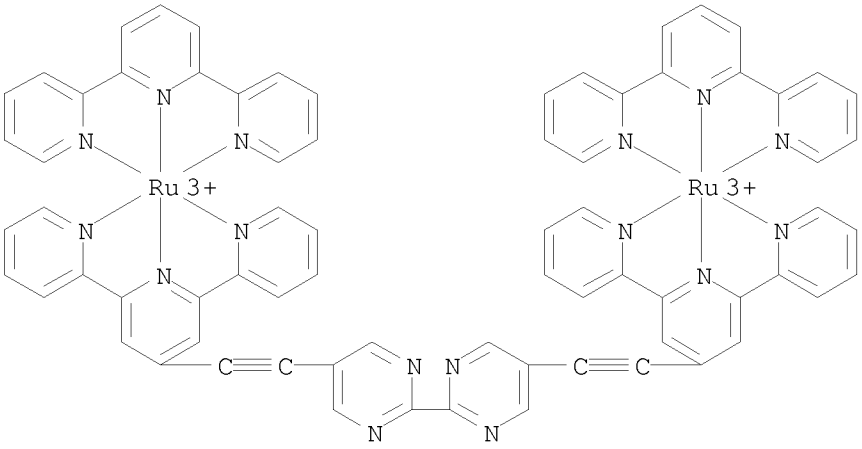
US 20050255157	A1	20051117	US 2005-126972	20050511
PRAI US 2004-569865P	P	20040511		

AB A sustained-release mucoadhesive vaginal pharmaceutical composition is provided comprising (a) an effective amount of at least one active pharmaceutical ingredient and (b) a hydrophilic matrix having mucoadhesive properties and capable of providing a sustained release of the active pharmaceutical ingredient, wherein the hydrophilic matrix contains a hydrophilic polymer having an average mol. weight of at least about 100,000. Also provided are solid oral dosage forms comprising the sustained release, mucoadhesive pharmaceutical compns. For example, a vaginal tablet contained clotrimazole 9.52, PVP K-25 2.5, colloidal silica 0.5, starch 32.19, lactose monohydrate 50.98, Polyox WSR-301 3.81, and Mg stearate 0.5 %.
IT 62973-76-6, Azanidazole
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(sustained-release mucoadhesive pharmaceuticals containing hydrophilic matrixes)
RN 62973-76-6 CAPLUS
CN 2-Pyrimidinamine, 4-[(1E)-2-(1-methyl-5-nitro-1H-imidazol-2-yl)ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.


H2N
N
N
E
N
N
Me
NO2

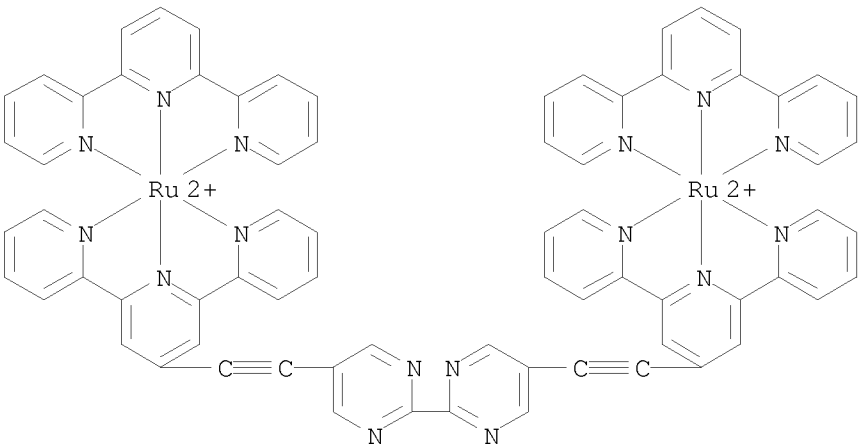
L8 ANSWER 26 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2005:730116 CAPLUS
DN 143:358956
TI Photophysical properties of binuclear ruthenium(II) bis(2,2':6',2''-terpyridine) complexes built around a central 2,2'-bipyrimidine receptor
AU Harriman, Anthony; Mayeux, Annabelle; Stroh, Christophe; Ziessel, Raymond
CS Molecular Photonics Laboratory, School of Natural Sciences-Chemistry, University of Newcastle, Newcastle-upon-Tyne, NE1 7RU, UK
SO Dalton Transactions (2005), (17), 2925-2932
CODEN: DTARAF; ISSN: 1477-9226
PB Royal Society of Chemistry
DT Journal
LA English
OS CASREACT 143:358956
AB A binuclear complex was synthesized having Ru(II) bis(2,2':6',2''-terpyridine) terminals attached to a central 2,2'-bipyrimidine unit via ethynylene groups. Cyclic voltammetry indicates that the substituted terpyridine is the most easily reduced subunit and the main chromophore involves charge transfer from the metal center to this ligand. The resultant metal-to-ligand, charge-transfer (MLCT) triplet state is weakly emissive and has a lifetime of 60 ns in deoxygenated solution at room temperature
The luminescence yield and lifetime increase with decreasing temperature in a manner that indicates the lowest-energy MLCT triplet couples to at least two higher-energy triplets. Cations can bind to the central bipyrimidine unit, forming both 1:1 and 1:2 (ligand to metal) complexes as confirmed by electrospray MS anal. The photophys. properties depend on the number of bound cations and on the nature of the cation. In the specific case of binding Zn(II) cations, the 1:1 complex has a triplet lifetime of 8.0 ns while that of the 1:2 complex is 1.8 ns. The 1:1 complexes formed with Ba2+ and Mg2+ are more luminescent than is the parent compound while the 1:2 complexes are much less luminescent. The coordinated cations raise the reduction potential of the central bipyrimidine unit and thereby increase the activation energy for coupling with the metal-centered state. Complexation also introduces a non-emissive intramol. charge-transfer (ICT) state that couples to the lowest-energy MLCT triplet and provides an addnl. nonradiative decay route. The triplet state of the 1:2 complex formed with added Zn2+ cations decays preferentially via this ICT state.
IT 736930-89-5
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(elec. potential of couple containing)
RN 736930-89-5 CAPLUS
CN Ruthenium(6+), [μ-[5,5'-bis[([2,2':6',2''-terpyridin]-4'-yl-κN1,κN1',κN1'')ethynyl]-2,2'-bipyrimidine]]bis(2,2':6',2''-terpyridine-κN1,κN1',κN1'')di- (9CI) (CA INDEX NAME)



IT 736930-81-7P
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
(preparation, luminescence, charge transfer transition, electrochem. oxidation
and reduction and complexation with metal cations)
RN 736930-81-7 CAPLUS
CN Ruthenium(4+), [μ-[5,5'-bis[([2,2':6',2''-terpyridin]-4'-yl-κN1,κN1',κN1'')ethynyl]-2,2'-bipyrimidine]]bis(2,2':6',2''-terpyridine-κN1,κN1',κN1'')di-, tetrakis[hexafluorophosphate(1-)] (9CI) (CA INDEX NAME)

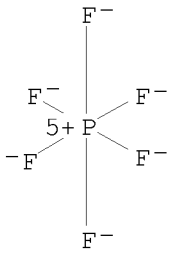
CM 1

CRN 736930-80-6
CMF C72 H46 N16 Ru2
CCI CCS

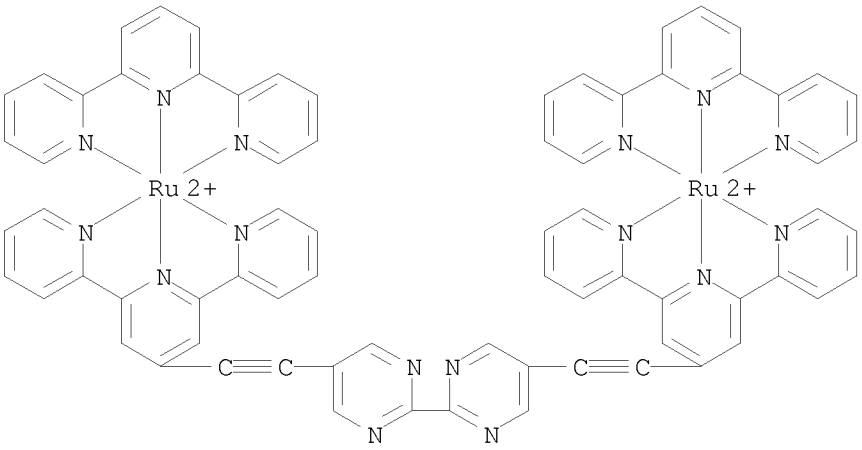


CM 2

CRN 16919-18-9
CMF F6 P
CCI CCS



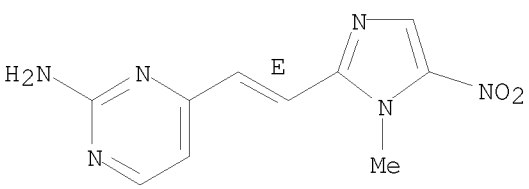
IT 736930-80-6D, complexes with metal ions
RL: CPS (Chemical process); FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); FORM (Formation, nonpreparative); PROC (Process)
(stability constant and cyclic voltammetry)
RN 736930-80-6 CAPLUS
CN Ruthenium(4+), [μ-[5,5'-bis[([2,2':6',2''-terpyridin]-4'-yl-κN1,κN1',κN1'')ethynyl]-2,2'-bipyrimidine]]bis(2,2':6',2''-terpyridine-κN1,κN1',κN1'')di- (9CI) (CA INDEX NAME)



RE.CNT 89 THERE ARE 89 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 27 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2005:708469 CAPLUS
DN 143:278397
TI A linear discrimination analysis based virtual screening of trichomonacidal lead-like compounds: Outcomes of in silico studies supported by experimental results
AU Meneses-Marcel, Alfredo; Marrero-Ponce, Yovani; Machado-Tugores, Yanetsy; Montero-Torres, Alina; Pereira, David Montero; Escario, Jose Antonio; Nogal-Ruiz, Juan Jose; Ochoa, Carmen; Aran, Vicente J.; Martinez-Fernandez, Antonio R.; Garcia Sanchez, Rory N.
CS Department of Parasitology, Chemical Bioactive Center, Central University of Las Villas, Villa Clara, 54830, Cuba
SO Bioorganic & Medicinal Chemistry Letters (2005), 15(17), 3838-3843
CODEN: BMCLE8; ISSN: 0960-894X
PB Elsevier B.V.
DT Journal
LA English
AB A computational (virtual) screening test to identify potential trichomonacidals has been developed. Mol. structures of trichomonacidal and non-trichomonacidal drugs were represented using stochastic and non-stochastic atom-based quadratic indexes and a linear discrimination anal. (LDA) was trained to classify mols. regarding their antiprotozoan activity. Validation tests revealed that our LDA-QSAR models recognize at least 88.24% of trichomonacidal lead-like compds. and suggest using this methodol. in virtual screening protocols. These classification functions were then applied to find new lead antitrichomonal compds. In this connection, the biol. assays of eight compds., selected by computational screening using the present models, give good results (87.50% of good classification). In general, most of the compds. showed high activity against Trichomonas vaginalis at the concentration of 100 μg/mL and low cytotoxicity to this concentration In particular, two heterocyclic derivs. (VA7-67 and VA7-69) maintained their efficacy at 10 μg/mL with an important trichomonacidal activity (100.00% of reduction), but it is remarkable that the compound VA7-67 did not show cytotoxic effects in macrophage cultivations. This result opens a door to a virtual study considering a higher variability of the structural core already evaluated, as well as of other chems. not included in this study.
IT 62973-76-6, Azanidazole
RL: BUU (Biological use, unclassified); PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(linear discrimination anal. based virtual screening of trichomonacidal lead-like compds. and outcomes of in silico studies supported by exptl. results)
RN 62973-76-6 CAPLUS
CN 2-Pyrimidinamine, 4-[(1E)-2-(1-methyl-5-nitro-1H-imidazol-2-yl)ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.



RE.CNT 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

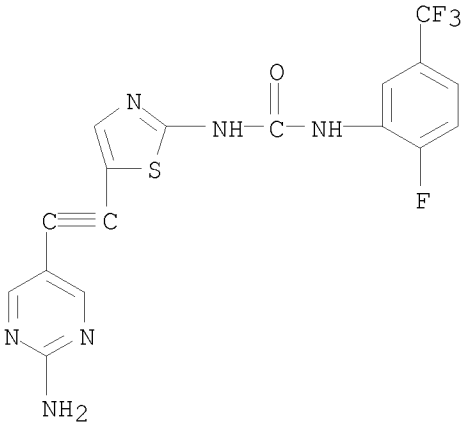
L8 ANSWER 28 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2005:588668 CAPLUS
DN 143:115557
TI Preparation of 2-aminopyrimidine derivatives as inhibitors of Tie2 receptor tyrosine kinases
IN Jones, Clifford David; Luke, Richard William Arthur; McCoull, William
PA Astrazeneca AB, Swed.; Astrazeneca UK Limited
SO PCT Int. Appl., 178 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005060970	A1	20050707	WO 2004-GB5337	20041220
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	EP 1737463	A1	20070103	EP 2004-806139	20041220
	R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR				
	CN 1917879	A	20070221	CN 2004-80041901	20041220
	JP 2007517007	T	20070628	JP 2006-546306	20041220
	US 20080108608	A1	20080508	US 2006-596745	20060622
	IN 2006MN00846	A	20070608	IN 2006-MN846	20060717
PRAI	GB 2003-30000	A	20031224		
	GB 2004-16849	A	20040729		
	WO 2004-GB5337	W	20041220		

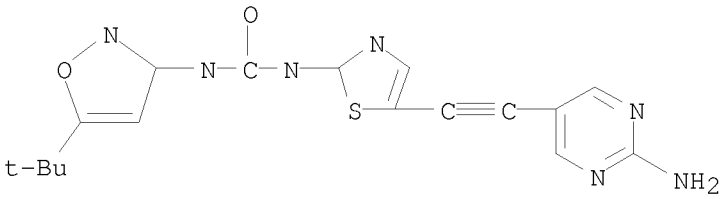
OS MARPAT 143:115557
AB Title compds. I [wherein R1, R2 = H, alkyl, alkanoyl; R3, R4 = H, alkyl, alkoxy; R5 = cyclopropyl, halo, cyano; m, n = 0-3; R6 = halo, oxo, cyano; etc., or salts thereof] were prepared as inhibitors of Tie2 receptor tyrosine kinases. Processes for the synthesis of I and some intermediates involved are claimed. For example, 2-amino-5-iodopyrimidine underwent Pd-catalyzed coupling with 3-ethynylaniline in the presence of CuI. The resultant substituted aniline was condensed with a carbamate, which was obtained from Ph chloroformate and 5-amino-3-methylisoxazole, to give urea II. This compound showed inhibition against Tie2 receptor tyrosine kinase in vitro and inhibition of autophosphorylation of Tie2 receptor tyrosine kinase with IC50 values of 19.871 μM and 0.337 μM, resp. Therefore, I and their pharmaceutical compns. have potential use in the production of an anti-angiogenic effect in a warm-blooded animal.
IT 857265-78-2P, N-[5-[(2-Aminopyrimidin-5-yl)ethynyl]-1,3-thiazol-2-yl]-N'-[2-fluoro-5-(trifluoromethyl)phenyl]urea 857265-82-8P, N-[5-[(2-Aminopyrimidin-5-yl)ethynyl]-1,3-thiazol-2-yl]-N'-(5-tert-butylisoxazol-3-yl)urea 857266-64-9P, N-[5-[(2-Aminopyrimidin-5-yl)ethynyl]-1,3-thiazol-2-yl]-N'-phenylurea 857266-65-0P, N-[5-[(2-Aminopyrimidin-5-yl)ethynyl]-1,3-thiazol-2-yl]-N'-(2,2-dimethyltetrahydro-2H-pyran-4-yl)urea 857266-67-2P,

N-[5-[(2-Aminopyrimidin-5-yl)ethynyl]-1,3-thiazol-2-yl]-N'-(3-cyclopropyl-1-methyl-1H-pyrazol-5-yl)urea 857266-70-7P, N-[5-[(2-Aminopyrimidin-5-yl)ethynyl]-1,3-thiazol-2-yl]-N'-(3-tert-butyl-1-methyl-1H-pyrazol-5-yl)urea
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(inhibitor; preparation of pyrimidine derivs. as inhibitors of Tie2 receptor tyrosine kinases)

RN 857265-78-2 CAPLUS
CN Urea, N-[5-[2-(2-amino-5-pyrimidinyl)ethynyl]-2-thiazolyl]-N'-[2-fluoro-5-(trifluoromethyl)phenyl]- (CA INDEX NAME)

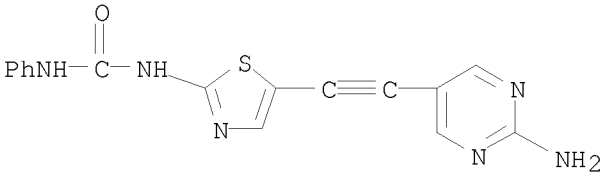


RN 857265-82-8 CAPLUS
CN Urea, N-[5-[2-(2-amino-5-pyrimidinyl)ethynyl]-2-thiazolyl]-N'-[5-(1,1-dimethylethyl)-3-isoxazolyl]- (CA INDEX NAME)

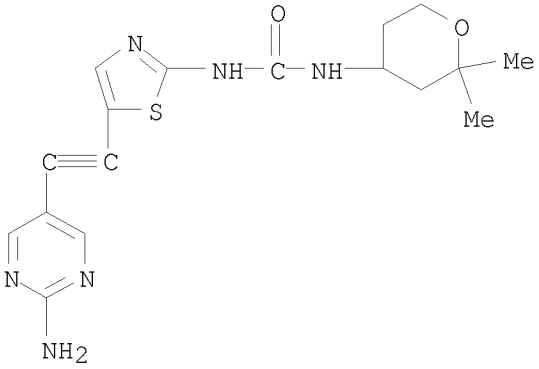


ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

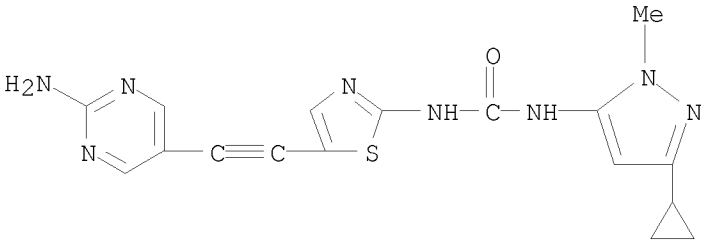
RN 857266-64-9 CAPLUS
CN Urea, N-[5-[2-(2-amino-5-pyrimidinyl)ethynyl]-2-thiazolyl]-N'-phenyl- (CA INDEX NAME)



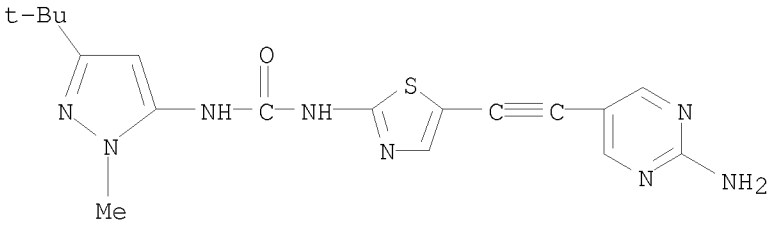
RN 857266-65-0 CAPLUS
CN Urea, N-[5-[2-(2-amino-5-pyrimidinyl)ethynyl]-2-thiazolyl]-N'-(tetrahydro-2,2-dimethyl-2H-pyran-4-yl)- (CA INDEX NAME)



RN 857266-67-2 CAPLUS
CN Urea, N-[5-[2-(2-amino-5-pyrimidinyl)ethynyl]-2-thiazolyl]-N'-(3-cyclopropyl-1-methyl-1H-pyrazol-5-yl)- (CA INDEX NAME)



RN 857266-70-7 CAPLUS
CN Urea, N-[5-[2-(2-amino-5-pyrimidinyl)ethynyl]-2-thiazolyl]-N'-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]- (CA INDEX NAME)



RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 29 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2005:158661 CAPLUS
DN 142:240460
TI Preparation of pyrimidine derivatives as ErbB kinase inhibitors
IN Reno, Michael John; Stevens, Kirk Lawrence; Waterson, Alex Gregory; Zhang, Yuemei
PA Smithkline Beecham Corporation, USA
SO PCT Int. Appl., 132 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

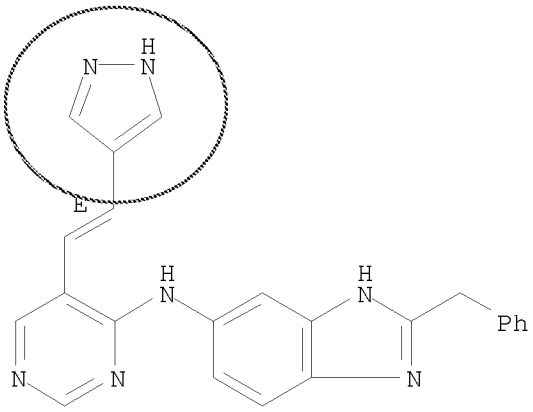
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005016914	A1	20050224	WO 2004-US26251	20040811
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	EP 1654251	A1	20060510	EP 2004-781004	20040811
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, HR				
	JP 2007502298	T	20070208	JP 2006-523388	20040811
	US 20060205740	A1	20060914	US 2006-568052	20060210
PRAI	US 2003-495180P	P	20030814		
	WO 2004-US26251	W	20040811		

OS CASREACT 142:240460; MARPAT 142:240460
AB Title compds. I [wherein A = alkenylene, alkynylene; R = alkylene; R1 = -(Z)-(Z1)m-(Z2)n; Z = hetero/aryl, hetero/arylene; Z1 = CH2 where m = 0-1; Z2 = OH and derivs., halo, CN, CONH2 and derivs. or heterocyclyl, where n = 0-1, etc.; R2 = H, alkyl; R3 = -(Q)-(Q1)r-(Q2); Q = hetero/arylene; Q1 = O, where r = 0-1; Q2 = arylalkyl, hetero/aryl; and their salts, solvates, and physiol. functional derivs.] were prepared as ErbB kinase inhibitors for treating cancer. Thus, reacting 2-benzyl-N-(5-vinylpyrimidin-4-yl)-1H-benzimidazol-5-amine (preparation given) with Ph iodide gave pyrimidine II in 8%. I showed inhibitory activity vs. EGFR, ErbB-2, and ErbB-4 protein tyrosine kinases with a pIC50 ≥ 5.0. I are useful in the treatment of diseases associated with inappropriate ErbB family kinase activity.
IT 845656-89-5P, 2-Benzyl-N-[5-[(E)-2-(1H-pyrazol-4-yl)ethenyl]pyrimidin-4-yl]-1H-benzimidazol-5-amine 845657-00-3P, 1-Benzyl-N-[5-[(E)-2-(1H-pyrazol-4-yl)ethenyl]pyrimidin-4-yl]-1H-indazol-5-amine 845657-17-2P, N-[3-Chloro-4-[(3-fluorobenzyl)oxy]phenyl]-5-[(E)-2-(1H-pyrazol-4-yl)ethenyl]pyrimidin-4-amine 845657-24-1P, N-[3-Chloro-4-[(3-fluorobenzyl)oxy]phenyl]-5-[(1-methyl-1H-imidazol-5-yl)ethynyl]pyrimidin-4-amine 845657-26-3P, N-[3-Chloro-4-[(3-fluorobenzyl)oxy]phenyl]-5-[(1H-pyrazol-4-yl)ethynyl]pyrimidin-4-amine 845657-28-5P, N-[3-Chloro-4-[(3-fluorobenzyl)oxy]phenyl]-5-[(1,3-thiazol-2-yl)ethynyl]pyrimidin-4-amine 845657-58-1P, [4-[[4-[[3-Chloro-4-[(3-fluorobenzyl)oxy]phenyl]amino]pyrimidin-5-yl]ethynyl]-1,3-thiazol-2-yl]methanol

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of pyrimidines as ErB kinase inhibitors)

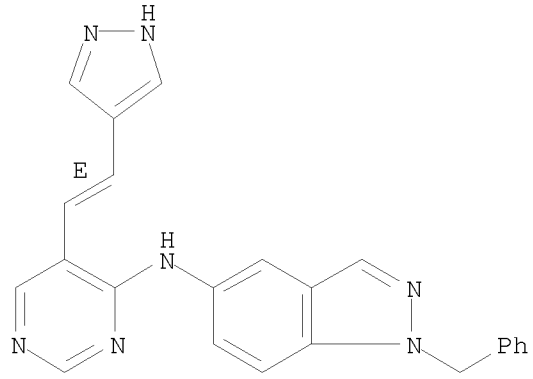
RN 845656-89-5 CAPLUS
CN 1H-Benzimidazol-6-amine, 2-(phenylmethyl)-N-[5-[(1E)-2-(1H-pyrazol-4-yl)ethenyl]-4-pyrimidinyl]- (CA INDEX NAME)

Double bond geometry as shown.



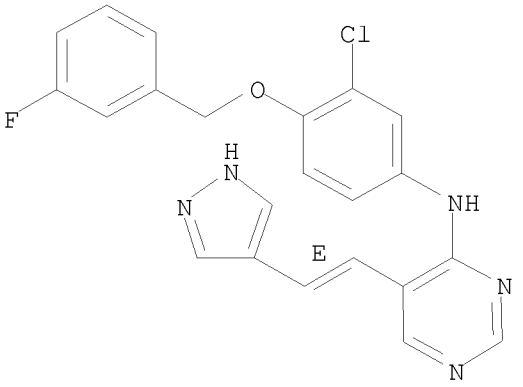
RN 845657-00-3 CAPLUS
CN 1H-Indazol-5-amine, 1-(phenylmethyl)-N-[5-[(1E)-2-(1H-pyrazol-4-yl)ethenyl]-4-pyrimidinyl]- (CA INDEX NAME)

Double bond geometry as shown.

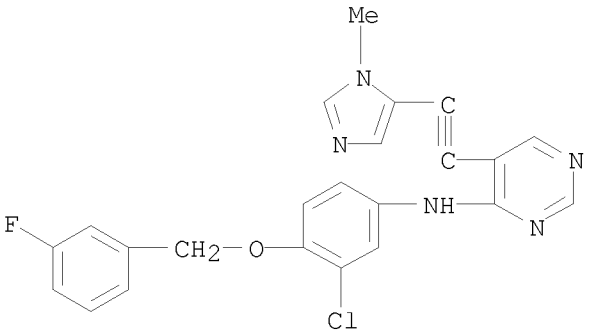


RN 845657-17-2 CAPLUS
CN 4-Pyrimidinamine, N-[3-chloro-4-[(3-fluorophenyl)methoxy]phenyl]-5-[(1E)-2-(1H-pyrazol-4-yl)ethenyl]- (CA INDEX NAME)

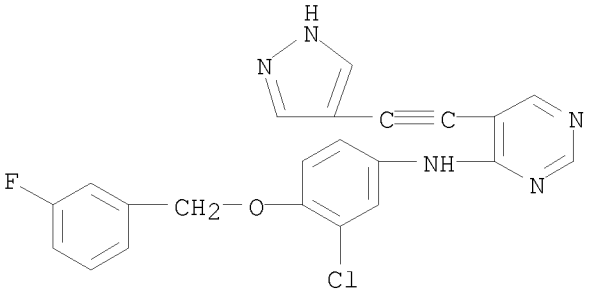
Double bond geometry as shown.



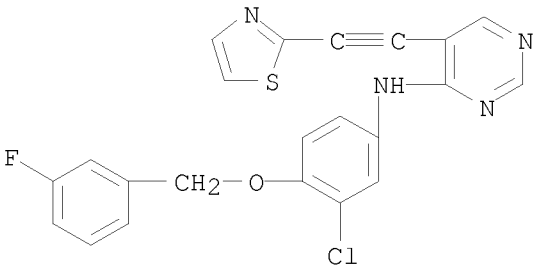
RN 845657-24-1 CAPLUS
CN 4-Pyrimidinamine, N-[3-chloro-4-[(3-fluorophenyl)methoxy]phenyl]-5-[2-(1-methyl-1H-imidazol-5-yl)ethynyl]- (CA INDEX NAME)



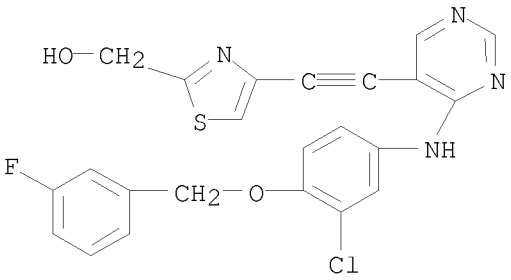
RN 845657-26-3 CAPLUS
CN 4-Pyrimidinamine, N-[3-chloro-4-[(3-fluorophenyl)methoxy]phenyl]-5-[2-(1H-pyrazol-4-yl)ethynyl]- (CA INDEX NAME)



RN 845657-28-5 CAPLUS
CN 4-Pyrimidinamine, N-[3-chloro-4-[(3-fluorophenyl)methoxy]phenyl]-5-[2-(2-thiazolyl)ethynyl]- (CA INDEX NAME)



RN 845657-58-1 CAPLUS
CN 2-Thiazolemethanol, 4-[2-[4-[[3-chloro-4-[(3-fluorophenyl)methoxy]phenyl]amino]-5-pyrimidinyl]ethynyl]- (CA INDEX NAME)



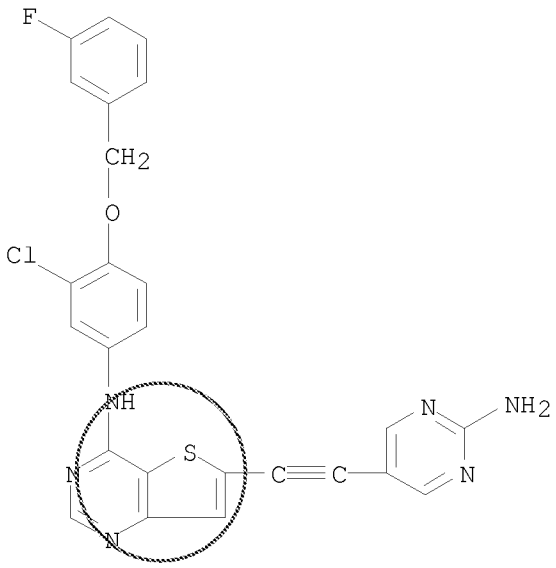
RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 30 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2004:1156446 CAPLUS
DN 142:74603
TI Preparation of thienopyrimidines as inhibitors of ErbB kinases
IN Badiang, Jennifer G.; Dickerson, Scott Howard; Donaldson, Kelly Horne; Hinkle, Kevin Wayne; Hornberger, Keith Robert; Petrov, Kimberly Glennon; Reno, Michael John; Stevens, Kirk Lawrence; Uehling, David Edward; Waterson, Alex Gregory
PA Smithkline Beecham Corporation, USA
SO PCT Int. Appl., 103 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2004112714	A2	20041229	WO 2004-US19388	20040617
WO 2004112714	A3	20050407		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRAI US 2003-479567P P 20030618
OS MARPAT 142:74603
AB Title compds. I [one of A1 and A2 = S, CH; R1 = heteroaryl, heteroarylene, arylene; R2 = H, alkyl; R3 = arylene, heteroarylene] are prepared For instance, N-[3-Chloro-4-[(3-fluorobenzyl)oxy]phenyl]-6-((pyridin-2-yl)ethynyl)thieno[2,3-d]pyrimidin-4-amine is prepared from 6-bromo-N-[3-chloro-4-[(3-fluorobenzyl)oxy]phenyl]thieno[2,3-d]pyrimidin-4-amine and 2-iodopyridine. Compds. of the invention have pIC50 of 5.5 or greater for EGFR kinase, ErbB-2 kinase and ErbB-4 kinase. I are useful for the treatment of diseases associated with inappropriate ErbB family kinase activity.
IT 815609-83-7P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of thienopyrimidines as inhibitors of ErbB kinases)
RN 815609-83-7 CAPLUS
CN Thieno[3,2-d]pyrimidin-4-amine, 6-[2-(2-amino-5-pyrimidinyl)ethynyl]-N-[3-chloro-4-[(3-fluorophenyl)methoxy]phenyl]- (CA INDEX NAME)


F
CH2
O
Cl
NH
N
S
C≡C
N
N
NH2
N

L8 ANSWER 31 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2004:566620 CAPLUS
DN 141:123650
TI Preparation of pyrimidine derivatives as Tie2 receptor tyrosine kinase inhibitors
IN Luke, Richard William Arthur
PA Astrazeneca Ab, Swed.; Astrazeneca Uk Limited
SO PCT Int. Appl., 70 pp.
CODEN: PIXXD2
DT Patent
LA English

Applicant's

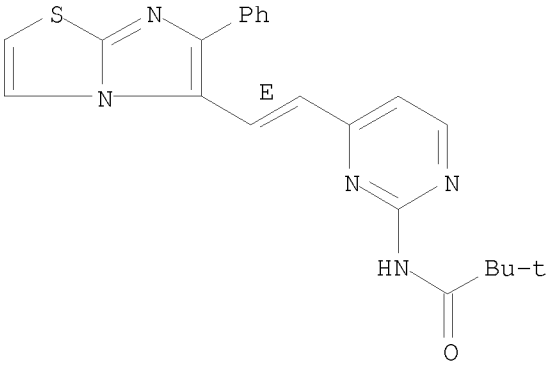
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004058776	A1	20040715	WO 2003-GB5568	20031219
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	CA 2508917	A1	20040715	CA 2003-2508917	20031219
	AU 2003295135	A1	20040722	AU 2003-295135	20031219
	EP 1575963	A1	20050921	EP 2003-786136	20031219
	EP 1575963	B1	20080507		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
	BR 2003017708	A	20051122	BR 2003-17708	20031219
	CN 1751052	A	20060322	CN 2003-80109832	20031219
	JP 2006515593	T	20060601	JP 2004-563345	20031219
	AT 394403	T	20080515	AT 2003-786136	20031219
	ZA 2005004827	A	20060426	ZA 2005-4827	20050613
	NO 2005002989	A	20050721	NO 2005-2989	20050617
	US 20060069109	A1	20060330	US 2005-540348	20050621
	MX 2005PA06921	A	20050818	MX 2005-PA6921	20050623
PRAI	GB 2002-30089	A	20021224		
	WO 2003-GB5568	W	20031219		

OS MARPAT 141:123650
AB The title compds. I [wherein L = a double bond and m = n = 1 or a triple bond and m = n = 0; G = O, S, or (un)substituted NH; Y = N or (un)substituted CH; Q1 = (un)substituted aryl or heteroaryl; R = H, NH2, OH, etc.; R1 = H, halo, CF3, etc.; R2 = H, halo, NH2, etc.; R3 = H, alkyl, CO2H, etc.; R4 = H, halo, CN, etc.] or pharmaceutically acceptable salts thereof are prepared For example, the compound II was prepared in a multi-step synthesis. I are useful as Tie2 receptor tyrosine kinase inhibitors in a warm-blooded animal such as man.
IT 723341-42-2P 723341-44-4P 723341-58-0P
723341-59-1P 723341-72-8P 723341-73-9P
723341-82-0P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(drug candidate; preparation of pyrimidine derivs. as Tie2 receptor tyrosine

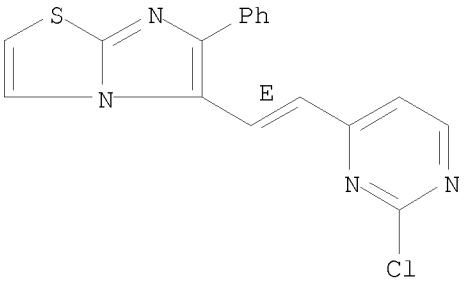
kinase inhibitors)
RN 723341-42-2 CAPLUS
CN Propanamide, 2,2-dimethyl-N-[4-[(1E)-2-(6-phenylimidazo[2,1-b]thiazol-5-yl)ethenyl]-2-pyrimidinyl]- (CA INDEX NAME)

Double bond geometry as shown.



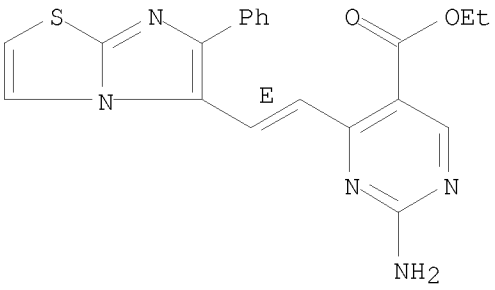
RN 723341-44-4 CAPLUS
CN Imidazo[2,1-b]thiazole, 5-[(1E)-2-(2-chloro-4-pyrimidinyl)ethenyl]-6-phenyl- (CA INDEX NAME)

Double bond geometry as shown.



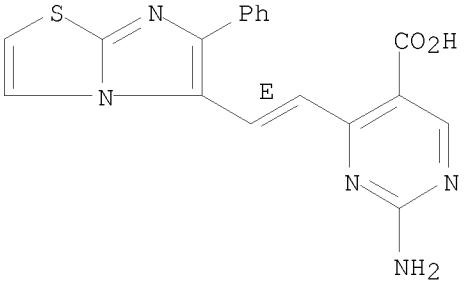
RN 723341-58-0 CAPLUS
CN 5-Pyrimidinecarboxylic acid, 2-amino-4-[(1E)-2-(6-phenylimidazo[2,1-b]thiazol-5-yl)ethenyl]-, ethyl ester (CA INDEX NAME)

Double bond geometry as shown.



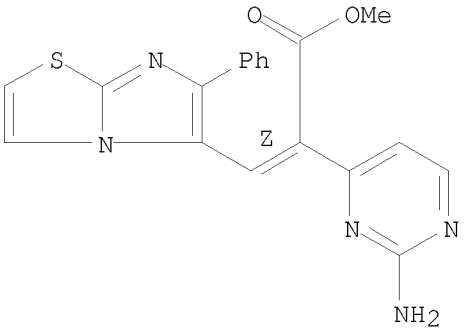
RN 723341-59-1 CAPLUS
CN 5-Pyrimidinecarboxylic acid, 2-amino-4-[(1E)-2-(6-phenylimidazo[2,1-b]thiazol-5-yl)ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.



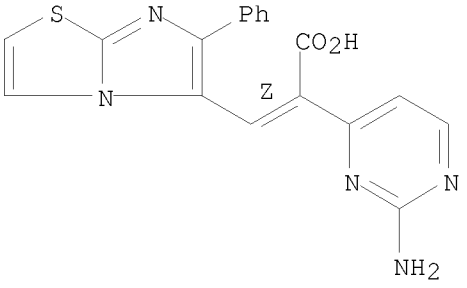
RN 723341-72-8 CAPLUS
CN 4-Pyrimidineacetic acid, 2-amino-α-[(6-phenylimidazo[2,1-b]thiazol-5-yl)methylene]-, methyl ester, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.

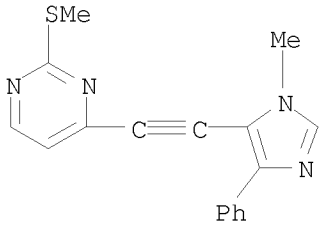


RN 723341-73-9 CAPLUS
CN 4-Pyrimidineacetic acid, 2-amino-α-[(6-phenylimidazo[2,1-b]thiazol-5-yl)methylene]-, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.

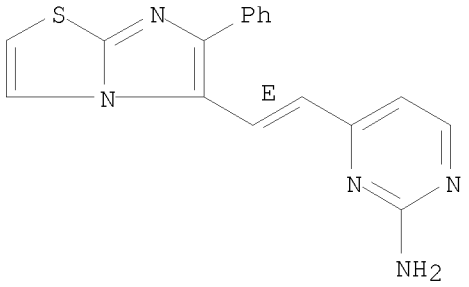


RN 723341-82-0 CAPLUS
CN Pyrimidine, 4-[2-(1-methyl-4-phenyl-1H-imidazol-5-yl)ethynyl]-2-(methylthio)- (CA INDEX NAME)



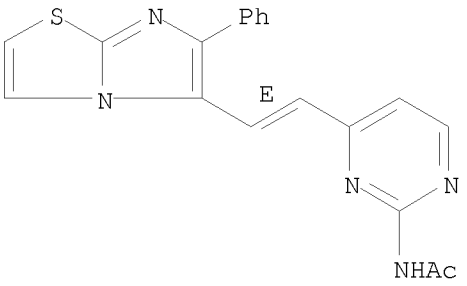
IT 723341-41-1P 723341-43-3P 723341-45-5P
723341-46-6P 723341-47-7P 723341-48-8P
723341-49-9P 723341-50-2P 723341-51-3P
723341-52-4P 723341-53-5P 723341-54-6P
723341-55-7P 723341-56-8P 723341-57-9P
723341-60-4P 723341-61-5P 723341-62-6P
723341-63-7P 723341-64-8P 723341-65-9P
723341-66-0P 723341-67-1P 723341-68-2P
723341-69-3P 723341-70-6P 723341-71-7P
723341-74-0P 723341-75-1P 723341-77-3P
723341-78-4P 723341-80-8P 723341-81-9P
723341-83-1P 723341-84-2P 723341-85-3P
724772-49-0P 724772-50-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of pyrimidine derivs. as Tie2 receptor tyrosine kinase inhibitors)
RN 723341-41-1 CAPLUS
CN 2-Pyrimidinamine, 4-[(1E)-2-(6-phenylimidazo[2,1-b]thiazol-5-yl)ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.



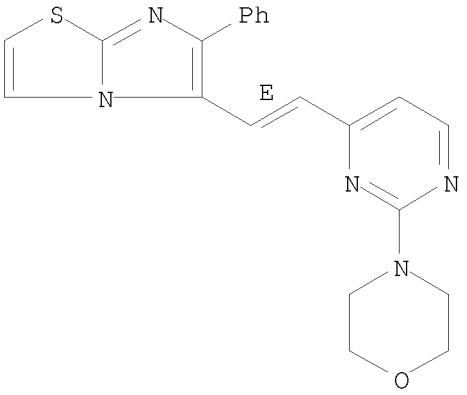
RN 723341-43-3 CAPLUS
CN Acetamide, N-[4-[(1E)-2-(6-phenylimidazo[2,1-b]thiazol-5-yl)ethenyl]-2-pyrimidinyl]- (CA INDEX NAME)

Double bond geometry as shown.



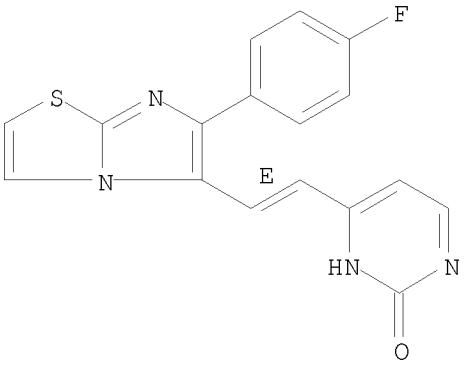
RN 723341-45-5 CAPLUS
CN Imidazo[2,1-b]thiazole, 5-[(1E)-2-[2-(4-morpholinyl)-4-pyrimidinyl]ethenyl]-6-phenyl- (CA INDEX NAME)

Double bond geometry as shown.



RN 723341-46-6 CAPLUS
CN 2(1H)-Pyrimidinone, 4-[(1E)-2-[6-(4-fluorophenyl)imidazo[2,1-b]thiazol-5-yl]ethenyl]- (CA INDEX NAME)

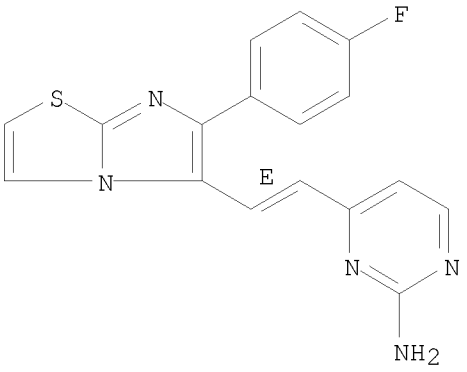
Double bond geometry as shown.



RN 723341-47-7 CAPLUS
CN 2-Pyrimidinamine, 4-[(1E)-2-[6-(4-fluorophenyl)imidazo[2,1-b]thiazol-5-

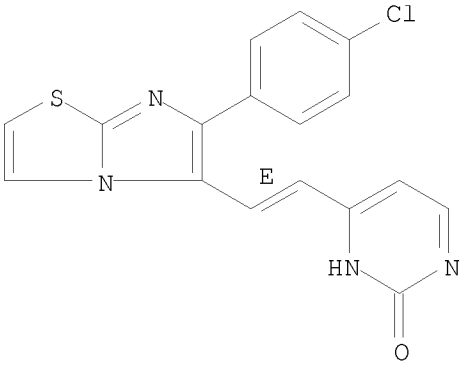
yl]ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.



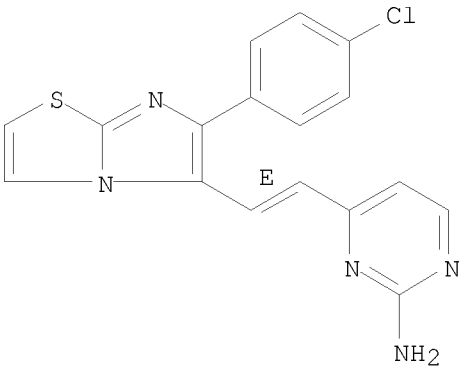
RN 723341-48-8 CAPLUS
CN 2(1H)-Pyrimidinone, 4-[(1E)-2-[6-(4-chlorophenyl)imidazo[2,1-b]thiazol-5-yl]ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.



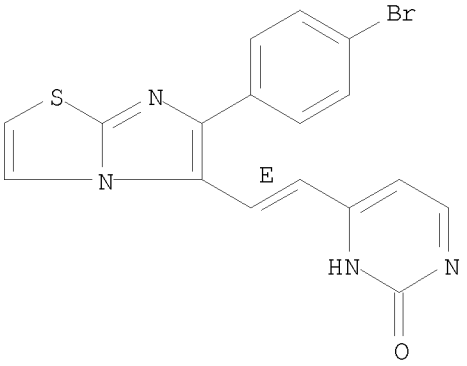
RN 723341-49-9 CAPLUS
CN 2-Pyrimidinamine, 4-[(1E)-2-[6-(4-chlorophenyl)imidazo[2,1-b]thiazol-5-yl]ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.



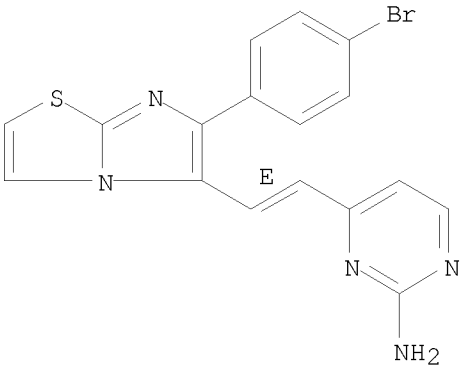
RN 723341-50-2 CAPLUS
CN 2(1H)-Pyrimidinone, 4-[(1E)-2-[6-(4-bromophenyl)imidazo[2,1-b]thiazol-5-yl]ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.



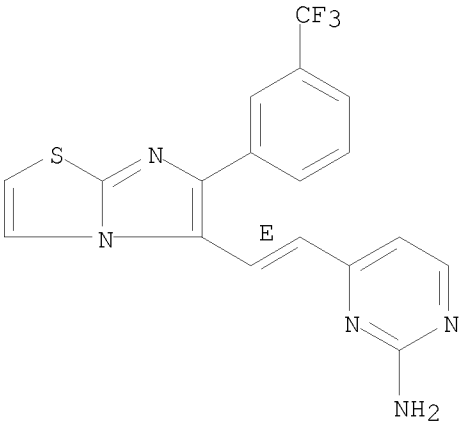
RN 723341-51-3 CAPLUS
CN 2-Pyrimidinamine, 4-[(1E)-2-[6-(4-bromophenyl)imidazo[2,1-b]thiazol-5-yl]ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.



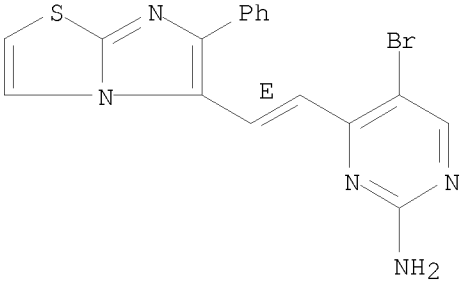
RN 723341-52-4 CAPLUS
CN 2-Pyrimidinamine, 4-[(1E)-2-[6-[3-(trifluoromethyl)phenyl]imidazo[2,1-b]thiazol-5-yl]ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.



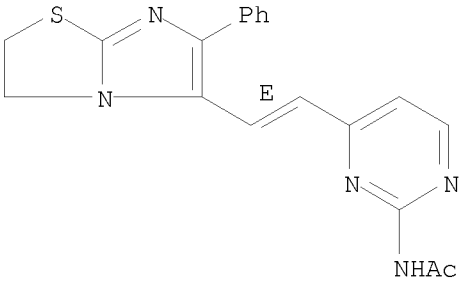
RN 723341-53-5 CAPLUS
CN 2-Pyrimidinamine, 5-bromo-4-[(1E)-2-(6-phenylimidazo[2,1-b]thiazol-5-yl)ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.



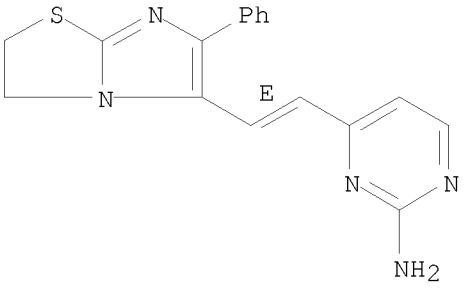
RN 723341-54-6 CAPLUS
CN Acetamide, N-[4-[(1E)-2-(2,3-dihydro-6-phenylimidazo[2,1-b]thiazol-5-yl)ethenyl]-2-pyrimidinyl]- (CA INDEX NAME)

Double bond geometry as shown.



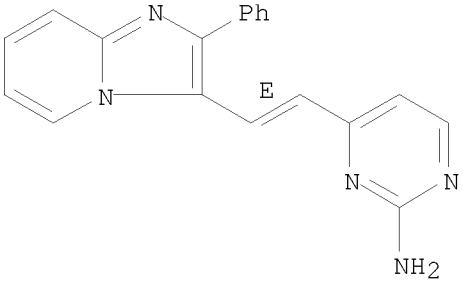
RN 723341-55-7 CAPLUS
CN 2-Pyrimidinamine, 4-[(1E)-2-(2,3-dihydro-6-phenylimidazo[2,1-b]thiazol-5-yl)ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.



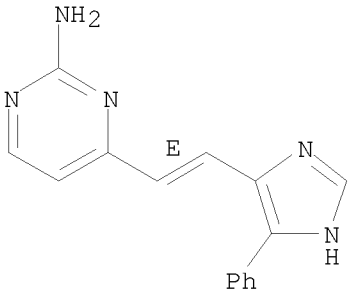
RN 723341-56-8 CAPLUS
CN 2-Pyrimidinamine, 4-[(1E)-2-(2-phenylimidazo[1,2-a]pyridin-3-yl)ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.



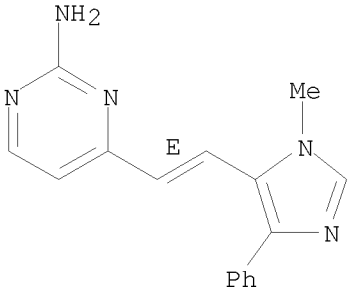
RN 723341-57-9 CAPLUS
CN 2-Pyrimidinamine, 4-[(1E)-2-(5-phenyl-1H-imidazol-4-yl)ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.



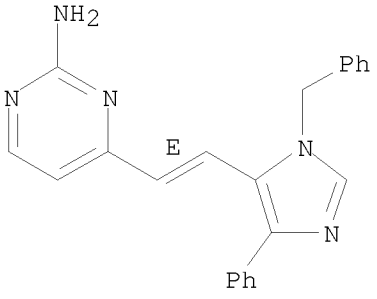
RN 723341-60-4 CAPLUS
CN 2-Pyrimidinamine, 4-[(1E)-2-(1-methyl-4-phenyl-1H-imidazol-5-yl)ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.



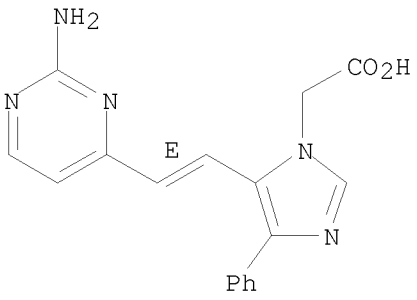
RN 723341-61-5 CAPLUS
CN 2-Pyrimidinamine, 4-[(1E)-2-[4-phenyl-1-(phenylmethyl)-1H-imidazol-5-yl]ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.



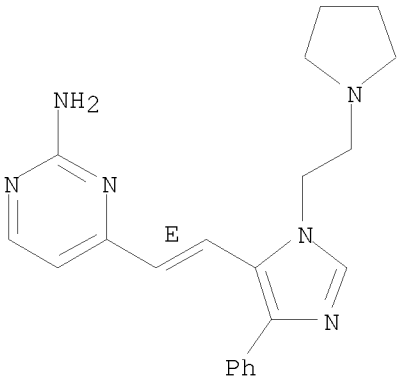
RN 723341-62-6 CAPLUS
CN 1H-Imidazole-1-acetic acid, 5-[(1E)-2-(2-amino-4-pyrimidinyl)ethenyl]-4-phenyl- (CA INDEX NAME)

Double bond geometry as shown.



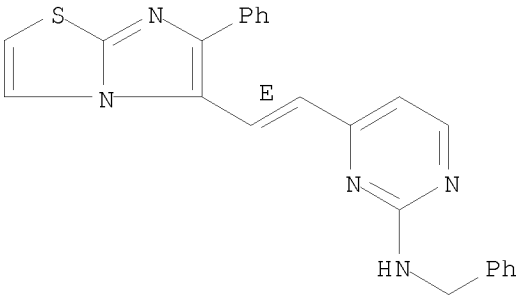
RN 723341-63-7 CAPLUS
CN 2-Pyrimidinamine, 4-[(1E)-2-[4-phenyl-1-[2-(1-pyrrolidinyl)ethyl]-1H-imidazol-5-yl]ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.



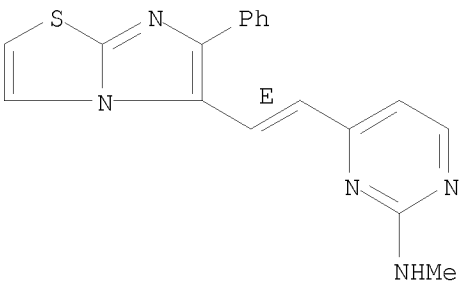
RN 723341-64-8 CAPLUS
CN 2-Pyrimidinamine, 4-[(1E)-2-(6-phenylimidazo[2,1-b]thiazol-5-yl)ethenyl]-N-(phenylmethyl)- (CA INDEX NAME)

Double bond geometry as shown.



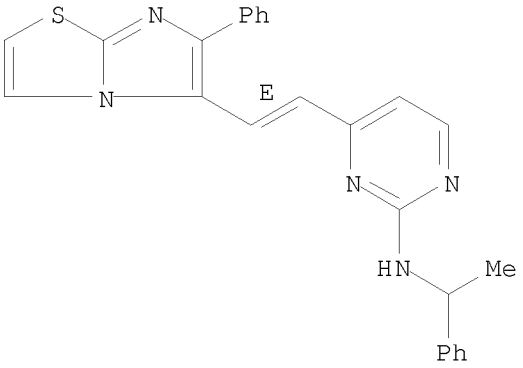
RN 723341-65-9 CAPLUS
CN 2-Pyrimidinamine, N-methyl-4-[(1E)-2-(6-phenylimidazo[2,1-b]thiazol-5-yl)ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.



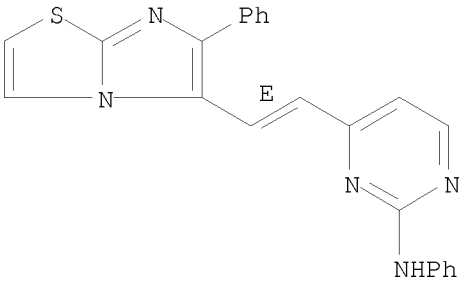
RN 723341-66-0 CAPLUS
CN 2-Pyrimidinamine, N-(1-phenylethyl)-4-[(1E)-2-(6-phenylimidazo[2,1-b]thiazol-5-yl)ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.



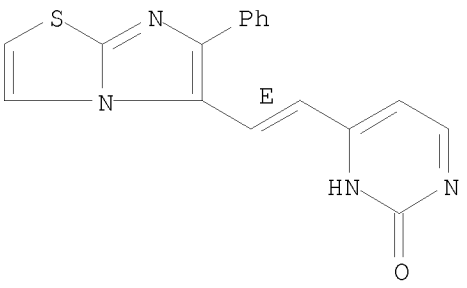
RN 723341-67-1 CAPLUS
CN 2-Pyrimidinamine, N-phenyl-4-[(1E)-2-(6-phenylimidazo[2,1-b]thiazol-5-yl)ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.



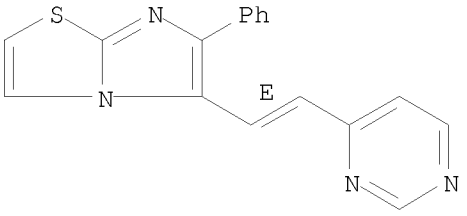
RN 723341-68-2 CAPLUS
CN 2(1H)-Pyrimidinone, 4-[(1E)-2-(6-phenylimidazo[2,1-b]thiazol-5-yl)ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.



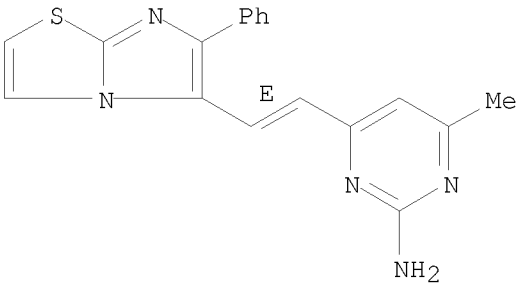
RN 723341-69-3 CAPLUS
CN Imidazo[2,1-b]thiazole, 6-phenyl-5-[(1E)-2-(4-pyrimidinyl)ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.



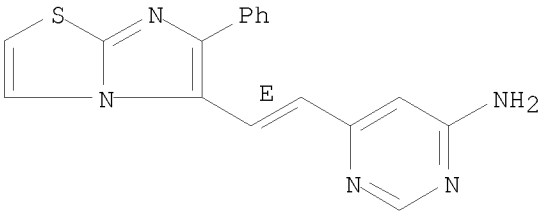
RN 723341-70-6 CAPLUS
CN 2-Pyrimidinamine, 4-methyl-6-[(1E)-2-(6-phenylimidazo[2,1-b]thiazol-5-yl)ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.



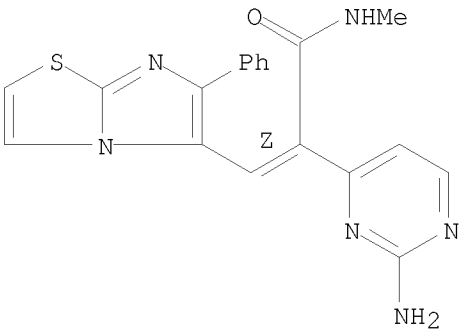
RN 723341-71-7 CAPLUS
CN 4-Pyrimidinamine, 6-[(1E)-2-(6-phenylimidazo[2,1-b]thiazol-5-yl)ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.

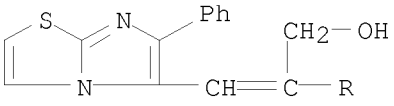


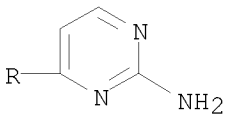
RN 723341-74-0 CAPLUS
CN 4-Pyrimidineacetamide, 2-amino-N-methyl-α-[(6-phenylimidazo[2,1-b]thiazol-5-yl)methylene]-, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



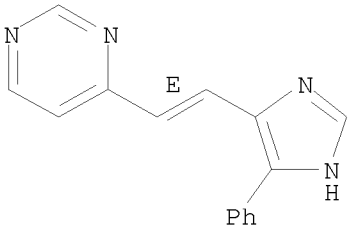
RN 723341-75-1 CAPLUS
CN 4-Pyrimidineethanol, 2-amino-β-[(6-phenylimidazo[2,1-b]thiazol-5-yl)methylene]- (CA INDEX NAME)





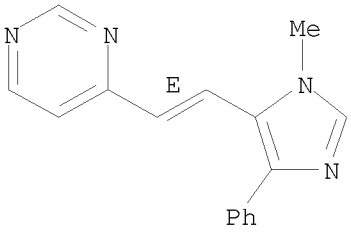
RN 723341-77-3 CAPLUS
CN Pyrimidine, 4-[(1E)-2-(5-phenyl-1H-imidazol-4-yl)ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.



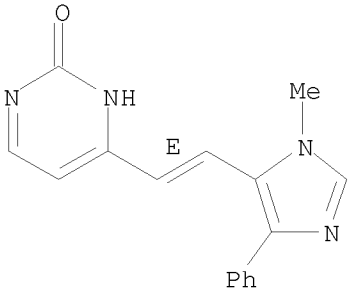
RN 723341-78-4 CAPLUS
CN Pyrimidine, 4-[(1E)-2-(1-methyl-4-phenyl-1H-imidazol-5-yl)ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.



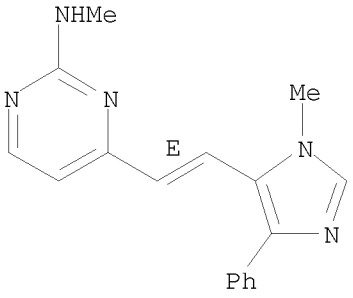
RN 723341-80-8 CAPLUS
CN 2(1H)-Pyrimidinone, 4-[(1E)-2-(1-methyl-4-phenyl-1H-imidazol-5-yl)ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.

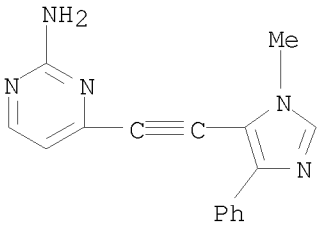


RN 723341-81-9 CAPLUS
CN 2-Pyrimidinamine, N-methyl-4-[(1E)-2-(1-methyl-4-phenyl-1H-imidazol-5-yl)ethenyl]- (CA INDEX NAME)

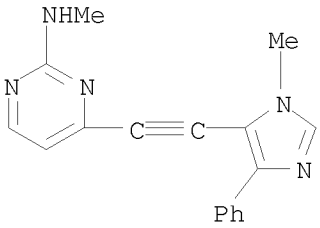
Double bond geometry as shown.



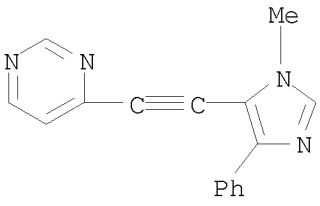
RN 723341-83-1 CAPLUS
CN 2-Pyrimidinamine, 4-[2-(1-methyl-4-phenyl-1H-imidazol-5-yl)ethynyl]- (CA INDEX NAME)



RN 723341-84-2 CAPLUS
CN 2-Pyrimidinamine, N-methyl-4-[2-(1-methyl-4-phenyl-1H-imidazol-5-yl)ethynyl]- (CA INDEX NAME)

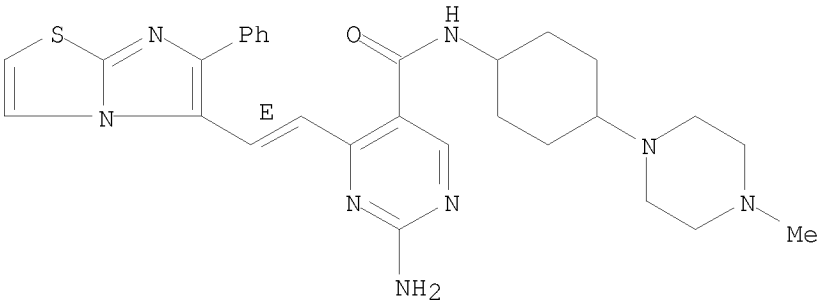


RN 723341-85-3 CAPLUS
CN Pyrimidine, 4-[2-(1-methyl-4-phenyl-1H-imidazol-5-yl)ethynyl]- (CA INDEX NAME)



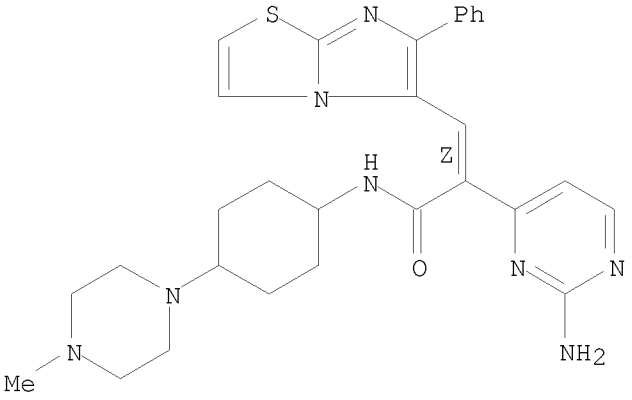
RN 724772-49-0 CAPLUS
CN 5-Pyrimidinecarboxamide, 2-amino-N-[4-(4-methyl-1-piperazinyl)cyclohexyl]-4-[(1E)-2-(6-phenylimidazo[2,1-b]thiazol-5-yl)ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.

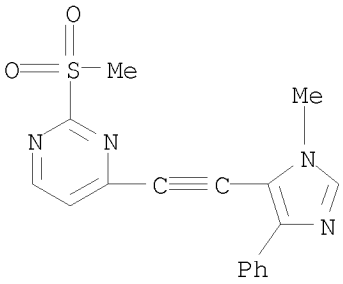


RN 724772-50-3 CAPLUS
CN 4-Pyrimidineacetamide, 2-amino-N-[4-(4-methyl-1-piperazinyl)cyclohexyl]-α-[(6-phenylimidazo[2,1-b]thiazol-5-yl)methylene]-, (αZ)- (CA INDEX NAME)

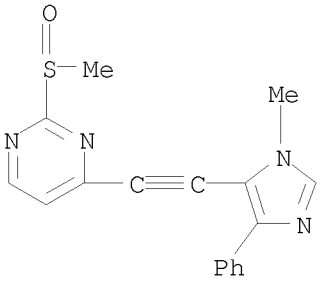
Double bond geometry as shown.



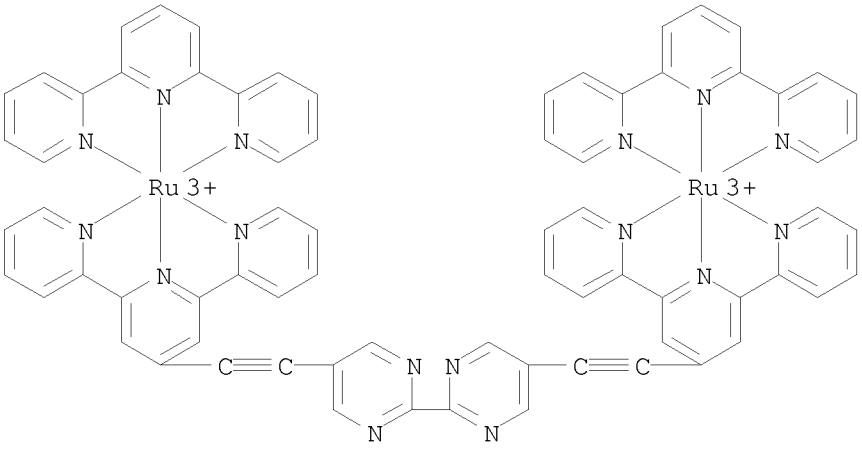
IT 723341-93-3P 723341-94-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of pyrimidine derivs. as Tie2 receptor tyrosine kinase inhibitors)
RN 723341-93-3 CAPLUS
CN Pyrimidine, 4-[2-(1-methyl-4-phenyl-1H-imidazol-5-yl)ethynyl]-2-(methylsulfonyl)- (CA INDEX NAME)



RN 723341-94-4 CAPLUS
CN Pyrimidine, 4-[2-(1-methyl-4-phenyl-1H-imidazol-5-yl)ethynyl]-2-(methylsulfinyl)- (CA INDEX NAME)



L8 ANSWER 32 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2004:479836 CAPLUS
DN 141:217786
TI cis-[Ru(2,2':6',2''-terpyridine)(DMSO)Cl2]: Useful Precursor for the Synthesis of Heteroleptic Terpyridine Complexes under Mild Conditions
AU Ziessel, Raymond; Grosshenny, Vincent; Hissler, Muriel; Stroh, Christophe
CS Laboratoire de Chimie Moleculaire, CNRS, Universite Louis Pasteur,Ecole de Chimie Polymeres, Materiaux de Strasbourg (ECPM), Strasbourg, 67087, Fr.
SO Inorganic Chemistry (2004), 43(14), 4262-4271
CODEN: INOCAJ; ISSN: 0020-1669
PB American Chemical Society
DT Journal
LA English
OS CASREACT 141:217786
AB [RuII(terpy)(DMSO)Cl2] complexes were synthesized as a 5/1 mixture of cis and trans isomers, and their reactivities with CO and with substituted 2,2':6',2''-terpyridine (terpy) moieties were studied. The structure of a trans isomer and its CO adduct were unambiguously assigned by spectroscopy and x-ray diffraction. The [Ru(terpy)(terpy-Br)]2+ complex prepared either from the cis-[RuII(terpy)(DMSO)Cl2] or from the cis-[RuII(terpy-Br)(DMSO)Cl2] precursor appeared to be reactive in cross-coupling reactions promoted by low-valent Pd(0) and is an attractive target for the stepwise synthesis of polynuclear complexes bearing vacant coordination sites (terpy-Br for 4'-bromo-2,2':6',2''-terpyridine). Several bipyridine, phenanthroline, and bipyrimidine complexes were prepared this way and their optical and redox properties determined and discussed.
IT 736930-89-5
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(elec. potential of couple containing)
RN 736930-89-5 CAPLUS
CN Ruthenium(6+), [μ-[5,5'-bis[([2,2':6',2''-terpyridin]-4'-yl-κN1,κN1',κN1'')ethynyl]-2,2'-bipyrimidine]]bis(2,2':6',2''-terpyridine-κN1,κN1',κN1'')di- (9CI) (CA INDEX NAME)



IT 736930-81-7P
RL: CPS (Chemical process); PEP (Physical, engineering or chemical

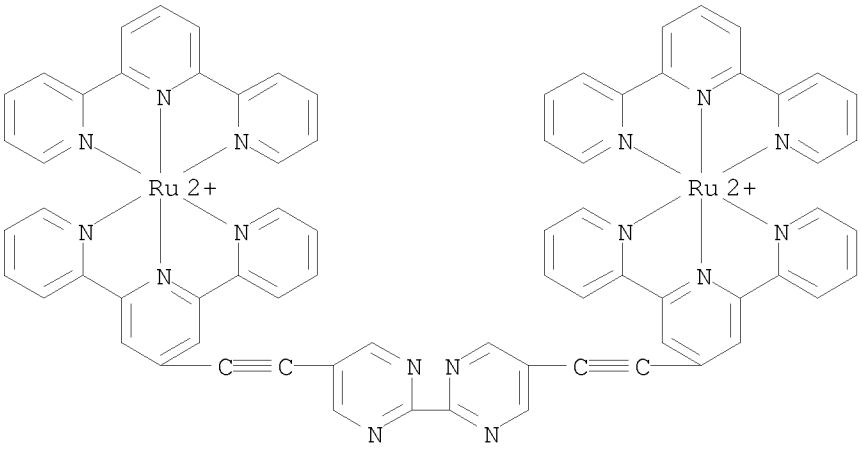
process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
(preparation and UV-visible spectra and electrochem. redox reactions)

RN 736930-81-7 CAPLUS

CN Ruthenium(4+), [μ-[5,5'-bis[([2,2':6',2''-terpyridin]-4'-yl-κN1,κN1',κN1'')ethynyl]-2,2'-bipyrimidine]]bis(2,2':6',2''-terpyridine-κN1,κN1',κN1'')di-, tetrakis[hexafluorophosphate(1-)] (9CI) (CA INDEX NAME)

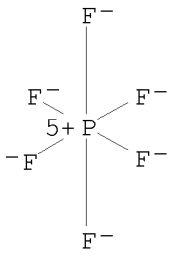
CM 1

CRN 736930-80-6
CMF C72 H46 N16 Ru2
CCI CCS



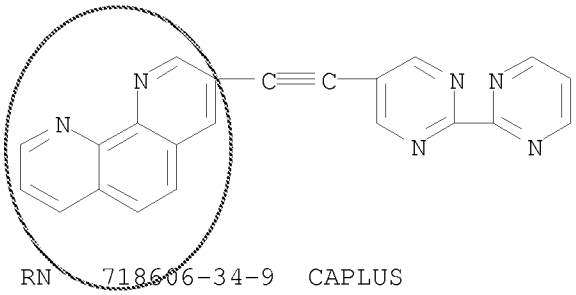
CM 2

CRN 16919-18-9
CMF F6 P
CCI CCS

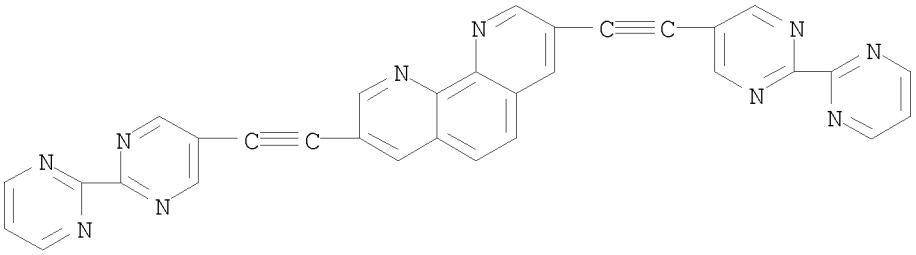


RE.CNT 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

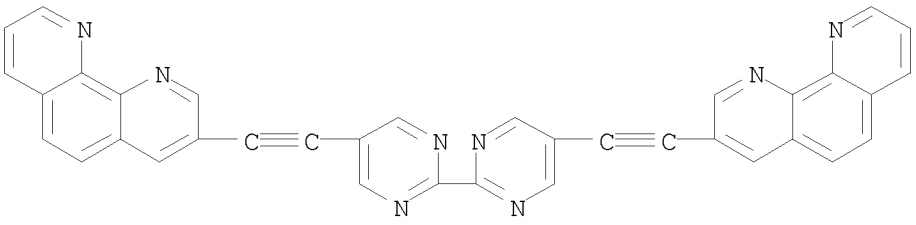
L8 ANSWER 33 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2004:363829 CAPLUS
DN 141:106434
TI Segmented multitopic ligands constructed from bipyrimidine, phenanthroline, and terpyridine modules
AU Ziessel, Raymond; Stroh, Christophe
CS Ecole de Chimie,Polymeres, Materiaux (ECPM), Laboratoire de Chimie Moleculaire, Universite Louis Pasteur (ULP), Strasbourg, 67087 02, Fr.
SO Tetrahedron Letters (2004), 45(21), 4051-4055
CODEN: TELEAY; ISSN: 0040-4039
PB Elsevier
DT Journal
LA English
OS CASREACT 141:106434
AB Starting from bromo-substituted 2,2'-bipyrimidine or 1,10-phenanthroline building blocks, the preparation in a first step of ethynyl grafted mols. allows the production in a second step of multitopic ligands by cross-coupling with difunctionalized chelating mols. Various combinations allow the interconnection of bipyrimidine to terpyridine, pyrene, or phenanthroline fragments. When two alkyne functions are present, a simple protocol gives a large variety of linear or bent ligands with an increasing number of nitrogen atoms. It was also possible to construct a linear complex capped at the periphery by ruthenium(II) centers and retaining an uncomplexed phenanthroline fragment in its core.
IT 718606-33-8P 718606-34-9P 718606-38-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of segmented multitopic ligands constructed from bipyrimidine, phenanthroline, and terpyridine modules)
RN 718606-33-8 CAPLUS
CN 1,10-Phenanthroline, 3-(2-[2,2'-bipyrimidin]-5-ylethynyl)- (CA INDEX NAME)



RN 718606-34-9 CAPLUS
CN 1,10-Phenanthroline, 3,8-bis(2-[2,2'-bipyrimidin]-5-ylethynyl)- (CA INDEX NAME)



RN 718606-38-3 CAPLUS
CN 1,10-Phenanthroline, 3,3'-([2,2'-bipyrimidine]-5,5'-diyldi-2,1-ethynediyl)bis- (9CI) (CA INDEX NAME)



RE.CNT 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 34 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2004:120856 CAPLUS
DN 140:163889
TI Preparation of condensed pyridines and pyrimidines as Tie2 receptor tyrosine kinase inhibitors and their anti-angiogenic effect
IN Luke, Richard William Arthur; Jones, Clifford David; McCoull, William; Hayter, Barry Raymond
PA Astrazeneca AB, Swed.; Astrazeneca UK Limited
SO PCT Int. Appl., 184 pp.
CODEN: PIXXD2
DT Patent
LA English
common inventor

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004013141	A1	20040212	WO 2003-GB3275	20030801
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	CA 2494421	A1	20040212	CA 2003-2494421	20030801
	AU 2003246972	A1	20040223	AU 2003-246972	20030801
	EP 1537112	A1	20050608	EP 2003-766443	20030801
	EP 1537112	B1	20060419		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
	BR 2003013078	A	20050712	BR 2003-13078	20030801
	CN 1688579	A	20051026	CN 2003-823754	20030801
	JP 2005538118	T	20051215	JP 2004-525533	20030801
	AT 323702	T	20060515	AT 2003-766443	20030801
	NO 2005000418	A	20050428	NO 2005-418	20050125
	ZA 2005000863	A	20060222	ZA 2005-863	20050128
	MX 2005PA01389	A	20050428	MX 2005-PA1389	20050203
	US 20050256140	A1	20051117	US 2005-523401	20050203
PRAI	GB 2002-18168	A	20020806		
	GB 2003-12356	A	20030530		
	WO 2003-GB3275	W	20030801		

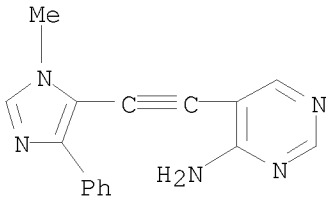
no ODP

OS MARPAT 140:163889
AB Title compds. I [wherein ACC = fused 5-membered heteroaryl ring; G = O, S and NH and derivs.; Z = N and CH and derivs.; Q1 = (un)substituted hetero/aryl; R1 = H, halo, CF3, CN, NO2, OH and derivs., NH2 and derivs., SH and derivs., N-alkyl/N,N-dialkyl/carbamoyl, alk(en/yn)yl, N-alkyl/alkanesulfonylamino, N-alkylsulfamoyl, etc.; R2 = H, , OH, halo, alkyl, alkoxy, formyl, alkyl/dialkyl/amino; R3 = independently as defined for R4, provided that R3 is not H, and when R3 is attached to a N atom in A, R3 is not halo; R4 = H, halo, CF3, OCF3, CN, NC, NO2, OH and derivs., SH and derivs., NH2 and derivs., formyl, CO2H and derivs. , carbamoyl, N-alkyl/N,N-dialkyl/sulfamoyl, alk(en/yn)yl, alkylthio, alkylsulfinyl, alkylsulfonyl, alkanoyl, alkanesulfonylamino, etc.] were prepared as Tie2 receptor tyrosine kinase inhibitors for use in the production of an anti-angiogenic effect in a warm-blooded animal. Thus, reacting II

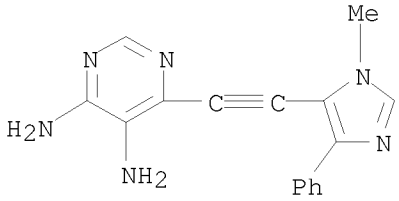
(preparation given) with 1-[(isocyanophenylmethyl)sulfonyl]-4-methylbenzene in the presence of piperazine/THF for 6 days gave the thieno[2,3-d]pyrimidine III in 48% yield. In a cellular assay, II inhibited autophosphorylation of the Tie2 receptor with an IC50 value of 2.2 μM. I are angiogenesis inhibitors for treating neoplasm (no data).

IT 655253-95-5P, 5-[(1-Methyl-4-phenyl-1H-imidazol-5-yl)ethynyl]pyrimidin-4-amine 655255-13-3P, 6-[(1-Methyl-4-phenyl-1H-imidazol-5-yl)ethynyl]pyrimidine-4,5-diamine
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of condensed pyridines and pyrimidines as Tie2 receptor tyrosine kinase inhibitors)

RN 655253-95-5 CAPLUS
CN 4-Pyrimidinamine, 5-[2-(1-methyl-4-phenyl-1H-imidazol-5-yl)ethynyl]- (CA INDEX NAME)



RN 655255-13-3 CAPLUS
CN 4,5-Pyrimidinediamine, 6-[2-(1-methyl-4-phenyl-1H-imidazol-5-yl)ethynyl]- (CA INDEX NAME)

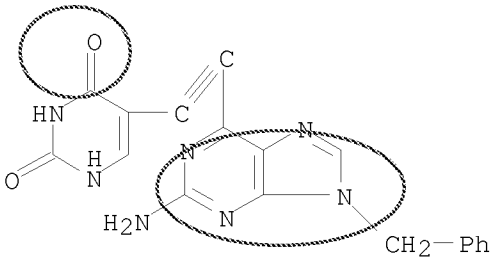


L8 ANSWER 35 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2003:1006984 CAPLUS
DN 140:42196
TI Preparation of alkynylpurine compounds
IN Hayashi, Taketo; Kawakami, Takehiko; Kumazawa, Hiroharu; Kotschy, Andras
PA Sumika Fine Chemicals Co., Ltd., Japan
SO PCT Int. Appl., 72 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003106458	A1	20031224	WO 2003-JP7317	20030610
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	JP 2004018453	A	20040122	JP 2002-175015	20020614
	CA 2489468	A1	20031224	CA 2003-2489468	20030610
	AU 2003238696	A1	20031231	AU 2003-238696	20030610
	EP 1515970	A1	20050323	EP 2003-733333	20030610
	EP 1515970	B1	20061018		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
	CN 1662536	A	20050831	CN 2003-813885	20030610
	AT 342902	T	20061115	AT 2003-733333	20030610
	US 20060100429	A1	20060511	US 2005-517599	20050914
PRAI	JP 2002-175015	A	20020614		
	WO 2003-JP7317	W	20030610		

OS CASREACT 140:42196; MARPAT 140:42196
AB The present invention relates to the preparation of alkynylpurine compds. I (R = alkyl, alkoxy, aryl, protected amino, halogen, H; R1 = R3C.tplbond.C, R3 = H, hydrocarbon optionally with substituents, aryl group optionally with substituents, heterocyclic group optionally with substituents, Me2COH; the other R1 = H; R2 = alkyl, sugar, amino-protecting group, H, which is attached to nitrogen atom at 7- or 9-position of purine nucleus, tetrahydropyran-2-yl, PhCH2) and II (R4 = H, hydrocarbon optionally with substituents, aryl optionally with substituents, heterocyclic group optionally with substituents; R5 = alkyl, alkoxy, aryl, optionally protected amino group, halogen, H; R6 = alkyl, sugar, amino-protecting group, H, which is attached to nitrogen atom at 7- or 9-position of purine nucleus). For example, reacting I (R1 = halogen, the other R1 = H, provided that when R = halogen, R1 = halogen with higher leaving ability than one represented by R) with Me2(OH)CC.tplbond.CH in the presence of metal catalyst and a base gave the desired compds.
IT 635709-65-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of alkynylpurine derivs.)
RN 635709-65-8 CAPLUS
CN 2,4(1H,3H)-Pyrimidinedione, 5-[2-[2-amino-9-(phenylmethyl)-9H-purin-6-

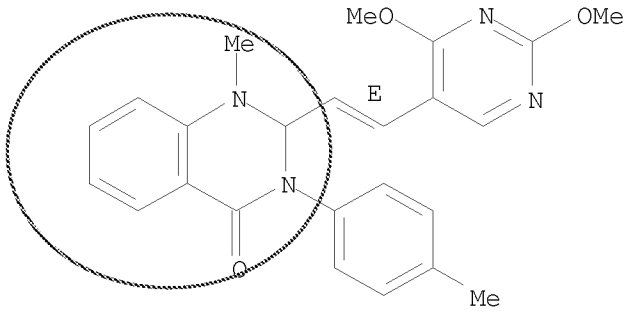
yl]ethynyl]- (CA INDEX NAME)



RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 36 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2001:538833 CAPLUS
DN 135:344437
TI Copper-catalyzed heteroannulation with alkynes: a general and highly regio- and stereoselective method for the synthesis of (E)-2-(2-arylvinyl) quinazolinones
AU Kundu, N. G.; Chaudhuri, G.
CS Department of Organic Chemistry, Indian Association for Cultivation of Science, Jadavpur, Calcutta, 700 032, India
SO Tetrahedron (2001), 57(31), 6833-6842
CODEN: TETRAB; ISSN: 0040-4020
PB Elsevier Science Ltd.
DT Journal
LA English
OS CASREACT 135:344437
AB A highly regio- and stereoselective procedure for the synthesis of 2-substituted-1,2,3,4-tetrahydroquinazolinones through a two-step procedure, e.g. (i) palladium-copper catalyzed C-arylation of terminal alkynes and (ii) copper-catalyzed cyclization of disubstituted alkynes, is described. 2-[Alkyl(2-propynyl)amino]-N-(4-methylphenyl)benzamides reacted with aryl iodides in the presence of (Ph3P)2PdCl2 (2.5 mol%), CuI (5 mol%), Et3N (5 equivalent) in CH3CN at rt for 16 h to yield disubstituted alkynes which could then be cyclized with CuI (20 mol%), K2CO3 (2.5 equivalent), Bu4NBr (1 equivalent) in CH3CN at 80°C for 16-24 h to yield 1-methyl(benzyl)-(E)-2-(2-arylvinyl)-3-p-tolyl-1,2,3,4-tetrahydro-4-quinazolinones in good yields. Said substituted [[(aminocarbonyl)phenyl]amino]alkynes included N-(4-methylphenyl)-2-[methyl(3-aryl-2-propynyl)amino]benzamide and N-(4-methylphenyl)-2-[(phenylmethyl)(3-aryl-2-propynyl)amino]benzamide derivs. Only in a few cases, benzodiazepinones were obtained in poor yield. The synthesis of novel uracil derivs. was also described.
IT 350603-11-1P 350603-15-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(regioselective, stereoselective preparation of (E)-2-(2-arylvinyl)quinazolinones via copper-catalyzed heteroannulation of [[(aryl)propynyl]amino]benzamide derivs.)
RN 350603-11-1 CAPLUS
CN 4(1H)-Quinazolinone, 2-[(1E)-2-(2,4-dimethoxy-5-pyrimidinyl)ethenyl]-2,3-dihydro-1-methyl-3-(4-methylphenyl)- (CA INDEX NAME)

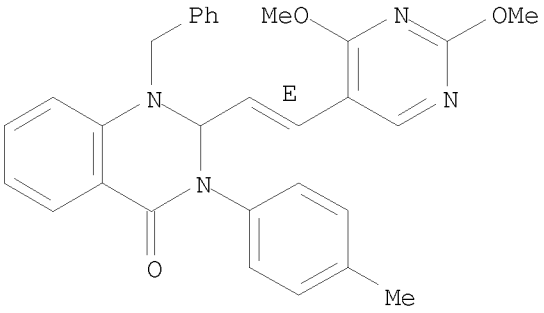
Double bond geometry as shown.



RN 350603-15-5 CAPLUS

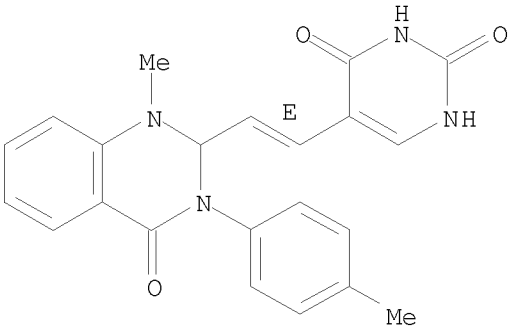
CN 4(1H)-Quinazolinone, 2-[(1E)-2-(2,4-dimethoxy-5-pyrimidinyl)ethenyl]-2,3-dihydro-3-(4-methylphenyl)-1-(phenylmethyl)- (CA INDEX NAME)

Double bond geometry as shown.



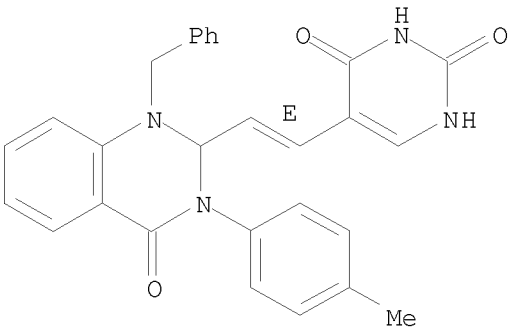
IT 371258-68-3P 371258-69-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(regioselective, stereoselective preparation of (E)-2-(2-arylvinyl)quinazolinones via copper-catalyzed heteroannulation of [[(aryl)propynyl]amino]benzamide derivs.)
RN 371258-68-3 CAPLUS
CN 2,4(1H,3H)-Pyrimidinedione, 5-[(1E)-2-[1,2,3,4-tetrahydro-1-methyl-3-(4-methylphenyl)-4-oxo-2-quinazolinyl]ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.



RN 371258-69-4 CAPLUS
CN 2,4(1H,3H)-Pyrimidinedione, 5-[(1E)-2-[1,2,3,4-tetrahydro-3-(4-methylphenyl)-4-oxo-1-(phenylmethyl)-2-quinazolinyl]ethenyl]- (CA INDEX NAME)

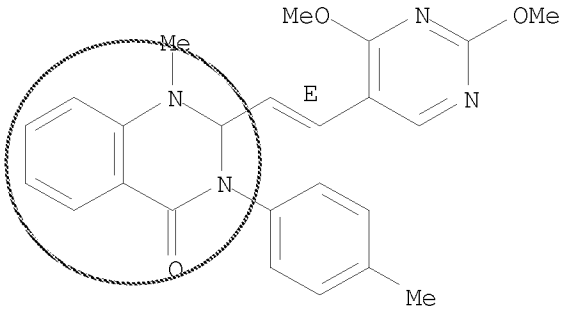
Double bond geometry as shown.



RE.CNT 78 THERE ARE 78 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

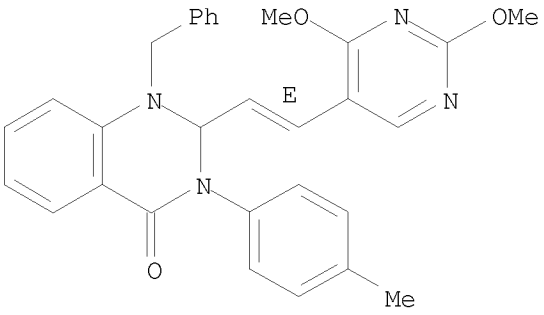
L8 ANSWER 37 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2001:246264 CAPLUS
DN 135:107296
TI Heteroannulation through copper catalysis: a novel and highly regio- and stereoselective cyclisation of alkynes leading to (E)-2-(2-arylvinyl)quinazolinones
AU Kundu, N. G.; Chaudhuri, G.
CS Department of Organic Chemistry, Indian Association for the Cultivation of Science, Calcutta, Jadavpur, 700 032, India
SO Tetrahedron Letters (2001), 42(15), 2883-2886
CODEN: TELEAY; ISSN: 0040-4039
PB Elsevier Science Ltd.
DT Journal
LA English
OS CASREACT 135:107296
AB 2-(Alkylprop-2-ynylamino)benzamides reacted with aryl iodides under Pd-Cu catalysis to yield disubstituted alkynes, which underwent a novel cyclization in the presence of CuI, K2CO3, and Bu4NBr in MeCN to yield (E)-1-alkyl-3-aryl-2-(2-arylvinyl)-4-quinazolinones in excellent yields instead of the expected benzodiazepinones.
IT 350603-11-1P 350603-15-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of (arylvinyl)quinazolinones by regio- and stereoselective cyclization of (alkynylamino)benzamides)
RN 350603-11-1 CAPLUS
CN 4(1H)-Quinazolinone, 2-[(1E)-2-(2,4-dimethoxy-5-pyrimidinyl)ethenyl]-2,3-dihydro-1-methyl-3-(4-methylphenyl)- (CA INDEX NAME)

Double bond geometry as shown.



RN 350603-15-5 CAPLUS
CN 4(1H)-Quinazolinone, 2-[(1E)-2-(2,4-dimethoxy-5-pyrimidinyl)ethenyl]-2,3-dihydro-3-(4-methylphenyl)-1-(phenylmethyl)- (CA INDEX NAME)

Double bond geometry as shown.

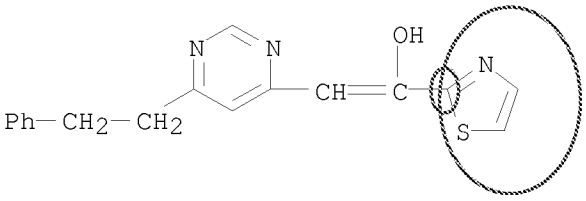


RE.CNT 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 38 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2001:185726 CAPLUS
DN 134:237486
TI Preparation of pyrimidines and pyridines derivatives as integrase inhibitors
IN Kawasuji, Takashi; Yoshinaga, Tomokazu
PA Shionogi & Co., Ltd., Japan
SO PCT Int. Appl., 155 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001017968	A1	20010315	WO 2000-JP5754	20000825
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	AU 2000067311	A	20010410	AU 2000-67311	20000825
	EP 1219607	A1	20020703	EP 2000-955030	20000825
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
PRAI	JP 1999-248206	A	19990902		
	WO 2000-JP5754	W	20000825		

OS MARPAT 134:237486
AB Title compds. [I; X is hydroxyl or the like; Y is C(:R2)R3R4 (wherein R2 and R3 are each oxygen or the like; and R4 is hydrogen or optionally substituted alkyl), optionally substituted heteroaryl, or the like; Z is hydrogen or the like; Z1 and Z3 are each independently a single bond, alkylene, or the like; Z2 is a single bond, alkylene, O, or the like; R1 is optionally substituted aryl, optionally substituted heteroaryl, or the like; p is 0 to 2; and A is an optionally substituted aromatic heterocycle], tautomers, prodrugs of both, pharmaceutically acceptable salts of them, or solvates are prepared and exhibit an integrase-inhibiting activity. Thus, the title compound II was prepared
IT 329983-05-3P 329983-11-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrimidines and pyridines derivs. as integrase inhibitors)
RN 329983-05-3 CAPLUS
CN 2-Thiazolemethanol, α-[[6-(2-phenylethyl)-4-pyrimidinyl]methylene]- (CA INDEX NAME)

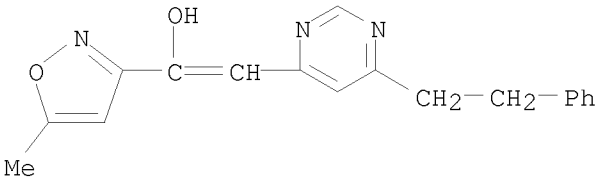


Two differences

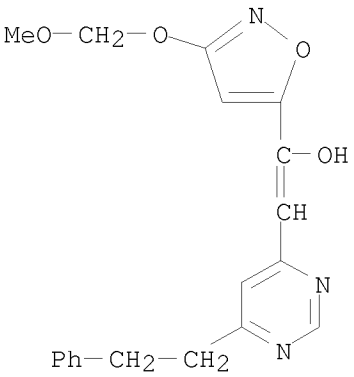
Q1 is cyclic in claims

Attachment via different position

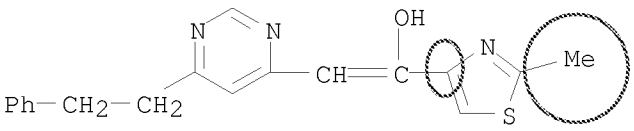
RN 329983-11-1 CAPLUS
CN 3-Isoxazolemethanol, 5-methyl-α-[[6-(2-phenylethyl)-4-pyrimidinyl]methylene]- (CA INDEX NAME)



IT 329983-06-4P
RL: RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of pyrimidines and pyridines derivs. as integrase inhibitors)
RN 329983-06-4 CAPLUS
CN 5-Isoxazolemethanol, 3-(methoxymethoxy)-α-[[6-(2-phenylethyl)-4-pyrimidinyl]methylene]- (CA INDEX NAME)

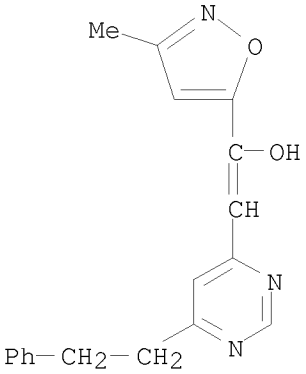


IT 329983-09-7P 329983-12-2P 329983-14-4P
329983-16-6P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrimidines and pyridines derivs. as integrase inhibitors)
RN 329983-09-7 CAPLUS
CN 4-Thiazolemethanol, 2-methyl-α-[[6-(2-phenylethyl)-4-pyrimidinyl]methylene]- (CA INDEX NAME)

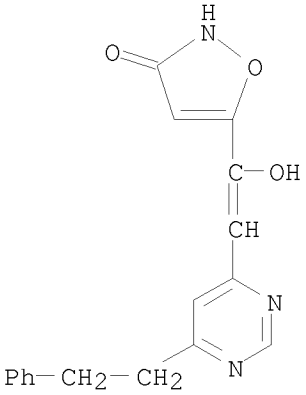


RN 329983-12-2 CAPLUS
CN 5-Isoxazolemethanol, 3-methyl-α-[[6-(2-phenylethyl)-4-

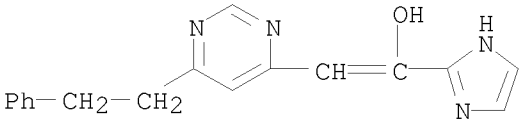
pyrimidinyl]methylene]- (CA INDEX NAME)



RN 329983-14-4 CAPLUS
CN 3(2H)-Isoxazolone, 5-[1-hydroxy-2-[6-(2-phenylethyl)-4-pyrimidinyl]ethenyl]- (CA INDEX NAME)



RN 329983-16-6 CAPLUS
CN 1H-Imidazole-2-methanol, α-[[6-(2-phenylethyl)-4-pyrimidinyl]methylene]- (CA INDEX NAME)

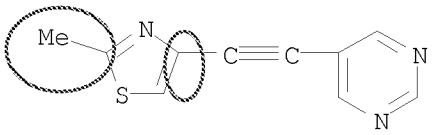


RE.CNT 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 39 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2001:167983 CAPLUS
DN 134:222706
TI Preparation of heterocyclic compounds as metabotropic glutamate receptor 5 (mGluR5) modulators
IN Cosford, Nicholas D. P.; McDonald, Ian A.; Bleicher, Leo Solomon; Cube, Rowena V.; Schweiger, Edwin J.; Vernier, Jean-Michel; Hess, Stephen D.; Varney, Mark A.; Munoz, Benito
PA Merck & Co., Inc., USA
SO PCT Int. Appl., 132 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 5

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001016121	A1	20010308	WO 2000-US23923	20000831
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	US 6956049	B1	20051018	US 1999-387135	19990831
	CA 2383524	A1	20010308	CA 2000-2383524	20000831
	EP 1214303	A1	20020619	EP 2000-957932	20000831
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
	JP 2003508390	T	20030304	JP 2001-519688	20000831
	AU 780009	B2	20050224	AU 2000-69482	20000831
PRAI	US 1999-387073	A2	19990831		
	US 1999-387135	A2	19990831		
	WO 2000-US23923	W	20000831		

OS MARPAT 134:222706
AB The title compds. I [ALB; A = 5-7 membered ring II (wherein at least one of W, X, Y and Z = (CR)p; p = 0-2, and the remainder of W, X, Y and Z = O, N, S; R = halo, (un)substituted aryl, heterocyclyl, etc.); L = (un)substituted alkenylene, alkynylene, azo; B = (un)substituted alkyl, cycloalkyl, heterocyclyl, etc.] and their pharmaceutically acceptable salts which are capable of modulating the activity of excitatory amino acid receptors such as metabotropic glutamate receptor, were prepared Thus, reacting 2-bromo-1,3-thiazole with phenylacetylene in the presence of CuI, Et3N and PdCl2(PPh3)2 in DME followed by treatment of the resulting 2-(phenylethynyl)-1,3-thiazole with p-TsOH afforded 2-(phenylethynyl)-1,3-thiazole, p-TsOH salt which showed IC50 of 0.1 nM - 10 μM in Ca+2 flux assay and analgesic efficacy in analgesic animal model (CFA model).
IT 329205-90-5P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of heterocyclic compds. as metabotropic glutamate receptor 5 (mGluR5) modulators)
RN 329205-90-5 CAPLUS
CN Pyrimidine, 5-[2-(2-methyl-4-thiazolyl)ethynyl]- (CA INDEX NAME)



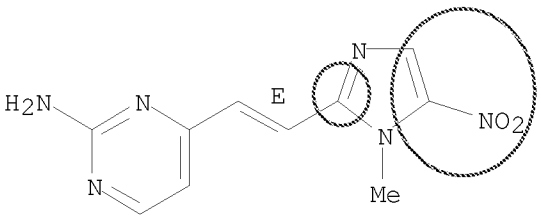
RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 40 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2000:462483 CAPLUS
DN 133:48920
TI Compositions for treating gastric ulcer and gastritis
IN Jiang, Enrong
PA Peop. Rep. China
SO Faming Zhuanli Shenqing Gongkai Shuomingshu, 6 pp.
CODEN: CNXXEV
DT Patent
LA Chinese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI CN 1205207	A	19990120	CN 1997-105966	19970711
PRAI CN 1997-105966		19970711		

AB The complex is composed of 5-nitroimidazole derivative 0.05-2.5 and Bi salt 0.1-12 parts, preferably 5-nitroimidazole derivative 0.55 and Bi salt 1.25 parts. The 5-nitroimidazole derivative is selected from metronidazole, azanidazole, aminitrozole, tinidazole, ornidazole, metronidazole benzoate, piperanidazole, secnidazole, and nimorazole; and the Bi salt from Bi oxycarbonate, bismuthyl nitrate, Bi subcitrate, and Bi subgallate.
IT 62973-76-6, Azanidazole
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(compns. for treating gastric ulcer and gastritis)
RN 62973-76-6 CAPLUS
CN 2-Pyrimidinamine, 4-[(1E)-2-(1-methyl-5-nitro-1H-imidazol-2-yl)ethenyl]-
(CA INDEX NAME)

Double bond geometry as shown.



L8 ANSWER 41 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2000:323247 CAPLUS
DN 132:344440
TI Preparation of ethylene derivatives pesticides.
IN Ogura, Tomoyuki; Murakami, Hiroshi; Numata, Akira; Miyachi, Rika; Miyake, Toshiro; Mimori, Norihiko; Takii, Shinji
PA Nissan Chemical Industries, Ltd., Japan
SO U.S., 110 pp., Cont.-in-part of Appl. No. PCT/JP97/01449.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 2

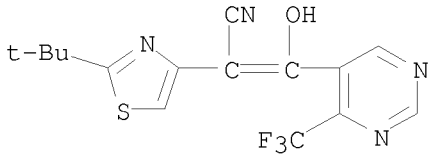
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6063734	A	20000516	US 1998-177501	19981023
	WO 9740009	A1	19971030	WO 1997-JP1440	19970424
	W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU				
	RW: GH, KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	ZA 9703563	A	19980115	ZA 1997-3563	19970424
	EP 1360901	A1	20031112	EP 2003-9790	19970424
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
	CN 1763003	A	20060426	CN 2005-10116118	19970424
	US 6462049	B1	20021008	US 2000-492321	20000127
	US 38188	E1	20030715	US 2001-983477	20011024
	US 20030216394	A1	20031120	US 2002-214258	20020808
	US 7037880	B2	20060502		
	JP 2003342262	A	20031203	JP 2003-109445	20030414
	JP 4054992	B2	20080305		
	US 20070049495	A1	20070301	US 2005-203341	20050815
	JP 2008001715	A	20080110	JP 2007-214182	20070820
PRAI	JP 1996-104878	A	19960425		
	JP 1996-145802	A	19960607		
	JP 1996-159346	A	19960620		
	JP 1997-28916	A	19970213		
	WO 1997-JP1440	A2	19970424		
	CN 1997-194041	A3	19970424		
	EP 1997-919686	A3	19970424		
	JP 1997-537934	A3	19970424		
	US 1998-177501	A3	19981023		
	US 2000-492321	A3	20000127		
	US 2002-214258	A1	20020808		

OS MARPAT 132:344440
AB The ethylene derivs. EQC:CA(OB) [Q = (un)unsubstituted Ph, 4-thiazolyl, 1- or 3-pyrazolyl, 1,3-oxazol-4-yl, pyridyl, etc.; E = Br, CN, CO2Me, etc.; A = 4-pyrazolyl, thiazolyl, etc.; B (in this abstract) = H, alkylcarbonyl, etc.], are prepared as agrochem. fungicides, insecticides, acaricides and marine antifouling agents.
IT 198072-29-6P 198072-63-8P 268744-45-2P
268749-39-9P
RL: AGR (Agricultural use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation as pesticide)

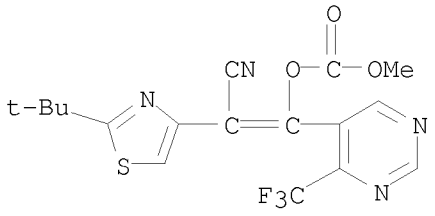
RN 198072-29-6 CAPLUS

CN 4-Thiazoleacetonitrile, 2-(1,1-dimethylethyl)-α-[hydroxy[4-(trifluoromethyl)-5-pyrimidinyl]methylene]- (CA INDEX NAME)



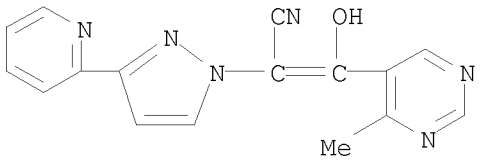
RN 198072-63-8 CAPLUS

CN Carbonic acid, 2-cyano-2-[2-(1,1-dimethylethyl)-4-thiazolyl]-1-[4-(trifluoromethyl)-5-pyrimidinyl]ethenyl methyl ester (CA INDEX NAME)



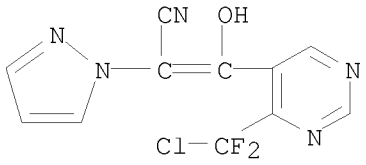
RN 268744-45-2 CAPLUS

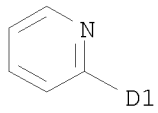
CN 1H-Pyrazole-1-acetonitrile, α-[hydroxy(4-methyl-5-pyrimidinyl)methylene]-3-(2-pyridinyl)- (CA INDEX NAME)



RN 268749-39-9 CAPLUS

CN 1H-Pyrazole-1-acetonitrile, α-[[4-(chlorodifluoromethyl)-5-pyrimidinyl]hydroxymethylene](2-pyridinyl)- (9CI) (CA INDEX NAME)





RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 42 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2000:289154 CAPLUS
DN 132:313708
TI Medicament for the topical treatment of inflammatory intestinal illnesses
IN Kist, Manfred; Otterbeck, Norbert
PA Falk Pharma G.m.b.H., Germany
SO Ger. Offen., 8 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI DE 19850445	A1	20000504	DE 1998-19850445	19981102
WO 2000025756	A2	20000511	WO 1999-EP8191	19991028
WO 2000025756	A3	20000727		

W: CA, IL, JP, US
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE

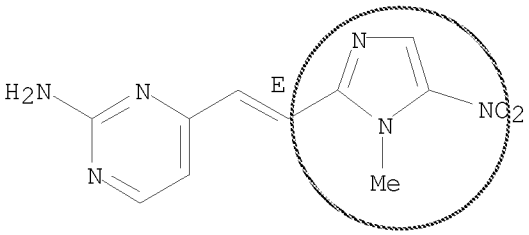
PRAI DE 1998-19850445 A 19981102

AB An antiprotozoal composition is provided which is taken orally, has a gastric juice-resistant coating, and acts topically directly on the intestinal site of inflammation. Administration of antiprotozoal agents locally in this manner minimizes the side effects observed when they are administered systemically, and diminishes the ED required. Thus, a mixture of metronidazole 5000, starch 1000, lactose 500, methylcellulose 200, SiO2 25, 40% aqueous Eudragit NE40D dispersion 750, and EtOH 500 g was kneaded, further mixed with 250 g Mg stearate, extruded, pelletized, and dried at 60°. The pellets were spray-coated with a solution of Eudragit S [350 g in 3500 g EtOH-H2O (8:2)] in which were suspended tri-Et citrate 35, talc 100, TiO2 125, and Mg stearate 50 g. These pellets released 0.9% of their metronidazole content in vitro in 120 min at pH 1.2, and 42.5% in 120 min at pH 6.8.

IT 62973-76-6, Azanidazole
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(medicament for topical treatment of inflammatory intestinal illnesses)

RN 62973-76-6 CAPLUS
CN 2-Pyrimidinamine, 4-[(1E)-2-(1-methyl-5-nitro-1H-imidazol-2-yl)ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.



RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 43 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1998:112204 CAPLUS
DN 128:184682
OREF 128:36399a,36402a
TI Bioadhesive complexes of polycarbophil and azole antifungal or antiprotozoal drugs
IN Saettone, Marco Fabrizio; Panichi, Luana; Giannaccini, Boris; Boldrini, Enrico; Bianchini, Pietro
PA Farmigea S.P.A., Italy
SO PCT Int. Appl., 36 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9805303	A1	19980212	WO 1997-IT187	19970725
	W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	AU 9738632	A	19980225	AU 1997-38632	19970725
	EP 918510	A1	19990602	EP 1997-935751	19970725
	EP 918510	B1	20020410		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO				
	AT 215815	T	20020415	AT 1997-935751	19970725
	US 20020012674	A1	20020131	US 1999-230863	19990202
	US 6423307	B2	20020723		
PRAI	IT 1996-RM559	A	19960802		
	WO 1997-IT187	W	19970725		

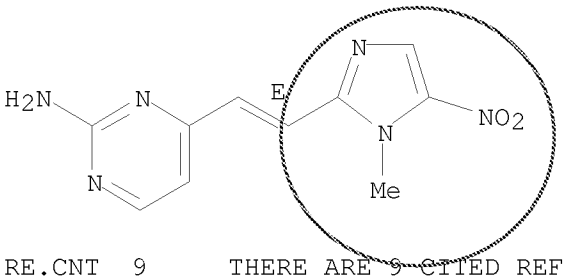
AB Mucoadhesive antimicrobial complexes of polycarbophil, i.e. a cross-linked polyacrylic acid with bioadhesive properties, and an imidazole or triazole derivative with antifungal or antiprotozoal activity, in its basic form, for use in the topical treatment of mucosal affections are disclosed. The complexes are obtainable by dissolving each of the two starting products in a common solvent, then joining together the two solns. in relative amts. such as to contain the same number of equivalent of the two starting products, evaporating the solvent and then drying and, if required, pulverizing and sieving the product so obtained. Particularly preferred are formulations in gel in propylene glycol comprising an econazole-polycarbophil or omoconazole-polycarbophil complex, with an excess of polycarbophil, together with pharmaceutically acceptable carrier and excipient substances, for use as sustained release antifungals for vaginal administration. A topical gel contained econazole base (in the complex) 3.00, polycarbophil (of which 1.12 g was complexed with econazole) 2.2, Me paraben 0.20, Pr paraben 0.02, and propylene glycol q.s. 100 g. The gel inhibited the growth of Candida albicans strains.

IT 62973-76-6D, Azanidazole, complexes with polycarbophil
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(bioadhesive complexes of polycarbophil and azole antifungal or antiprotozoal drugs)

RN 62973-76-6 CAPLUS

CN 2-Pyrimidinamine, 4-[(1E)-2-(1-methyl-5-nitro-1H-imidazol-2-yl)ethenyl]-
(CA INDEX NAME)

Double bond geometry as shown.

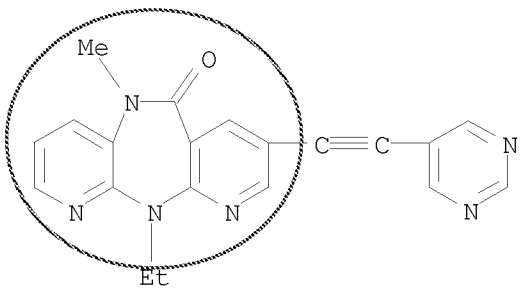


RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 44 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1998:31142 CAPLUS
DN 128:114968
OREF 128:22545a,22548a
TI Preparation of 8-aralkyl-5,11-dihydro-6H-dipyrido[3,2-b:2',3'-e][1]diazepines for treatment of HIV-1 infection.
IN Cywin, Charles L.; Hoermann, Maryann; Klunder, Janice M.
PA Boehringer Ingelheim Pharmaceuticals, Inc., USA
SO U.S., 39 pp.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 5705499	A	19980106	US 1996-710996	19960925
PRAI US 1996-710996		19960925		

OS MARPAT 128:114968
AB Title compds. [I; A = chain of 1-3 atoms, cyclopropylene, oxiranylene; Ar = (substituted) 5-6 membered (hetero)aryl; R1 = H, alkyl, fluoroalkyl, alkenylmethyl, alkynylmethyl, (substituted) aryl, arylmethylalkanoyl, thioalkanoyl, alkylsulfonyl, etc.; Z = O, S, NCN, alkoximino; R2 = H, alkyl, fluoroalkyl, cycloalkyl, oxetanyl, thietanyl, tetrahydrofuryl, alkenylmethyl, alkynylmethyl, alkoxyalkyl, alkylthioalkyl, alkanoyl, cyano, cyanoalkyl, hydroxyalkyl, acyloxyalkyl, etc.; R3 = H, alkyl, alkenyl, alkynyl, trihalomethyl, hydroxyalkyl, alkoxyalkyl, alkylthioalkyl, halo; R4 = H, Me, halo; R5 = H; R3R4 or R4R5 = cycloalkyl; with provisos], were prepared Thus, 2-chloro-5,11-dihydro-11-ethyl-5-methyl-8-[2-(pyrid-4-yloxy)ethyl]-6H-dipyrido[3,2-b:2',3'-e][1,4]diazepin-6-one (preparation given) showed an IC50 = 0.03 μM in the syncytia assay using HIV-1 in CD4+ T-cells.
IT 189393-30-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of aralkyldihydrodipyridodiazepines for treatment of HIV-1 infection)
RN 189393-30-4 CAPLUS
CN 6H-Dipyrido[3,2-b:2',3'-e][1,4]diazepin-6-one, 11-ethyl-5,11-dihydro-5-methyl-8-(5-pyrimidinylethynyl)- (9CI) (CA INDEX NAME)



RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 45 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1997:717885 CAPLUS
DN 127:331484
OREF 127:65101a,65104a
TI Preparation of ethylene derivatives as pest controlling agents
IN Ogura, Tomoyuki; Murakami, Hiroshi; Numata, Akira; Miyachi, Rika
PA Nissan Chemical Industries, Ltd., Japan; Ogura, Tomoyuki;
SO PCT Int. Appl., 423 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9740009	A1	19971030	WO 1997-JP1440	19970424
	W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU				
	RW: GH, KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	CA 2252536	A1	19971030	CA 1997-2252536	19970424
	AU 9724071	A	19971112	AU 1997-24071	19970424
	AU 736854	B2	20010802		
	ZA 9703563	A	19980115	ZA 1997-3563	19970424
	EP 913392	A1	19990506	EP 1997-919686	19970424
	EP 913392	B1	20030702		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
	CN 1216530	A	19990512	CN 1997-194041	19970424
	BR 9709126	A	20000111	BR 1997-9126	19970424
	TW 449460	B	20010811	TW 1997-86105307	19970424
	AT 244219	T	20030715	AT 1997-919686	19970424
	EP 1360901	A1	20031112	EP 2003-9790	19970424
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
	PT 913392	T	20031128	PT 1997-919686	19970424
	ES 2201293	T3	20040316	ES 1997-919686	19970424
	CN 1763003	A	20060426	CN 2005-10116118	19970424
	US 6063734	A	20000516	US 1998-177501	19981023
	KR 2000010635	A	20000225	KR 1998-708544	19981024
	US 6462049	B1	20021008	US 2000-492321	20000127
	US 38188	E1	20030715	US 2001-983477	20011024
	US 20030216394	A1	20031120	US 2002-214258	20020808
	US 7037880	B2	20060502		
	JP 2003342262	A	20031203	JP 2003-109445	20030414
	JP 4054992	B2	20080305		
	US 20070049495	A1	20070301	US 2005-203341	20050815
	JP 2008001715	A	20080110	JP 2007-214182	20070820
PRAI	JP 1996-104878	A	19960425		
	JP 1996-145802	A	19960607		
	JP 1996-159346	A	19960620		
	JP 1997-28916	A	19970213		
	CN 1997-194041	A3	19970424		
	EP 1997-919686	A3	19970424		
	JP 1997-537934	A3	19970424		

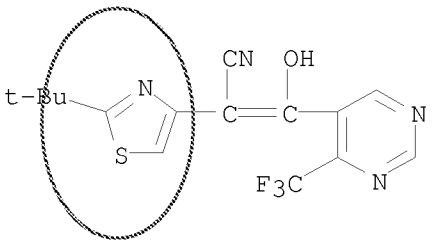
WO 1997-JP1440 W 19970424
US 1998-177501 A3 19981023
US 2000-492321 A3 20000127
US 2002-214258 A1 20020808

OS MARPAT 127:331484

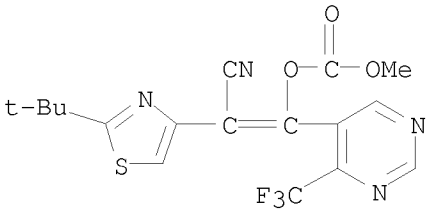
AB Phenylheterocyclylethylene derivs. of general formula EC(Q):C(A)OB[A, Q = (un)substituted Ph, naphthyl, or heterocyclyl, particularly, 4-thiazolyl, 1- or 3-pyrazolyl, 1,3-oxazol-4-yl, Ph, or pyridyl; E = cyano, or the like; A is 4-pyrazolyl, thiazolyl or the like; B = H, C1-4 (halo)alkyl, C2-4 alkoxyalkyl, MeSCH2, MeOCH2CH2OCH2, (un)substituted phenyl-C1-4 alkyl or benzoyl-C1-4 alkyl, tetrahydropyranyl, Me3Si, C1-4 alkylsulfonyl, etc.; E = optionally C1-4 alkyl or C1-4 haloalkyl-substituted heterocyclyl, C2-4 alkynyl, (un)substituted phenylethynyl, C1-4 haloalkyl, cyano, NO2, N3, CHO, (un)substituted COPh, etc.], which are useful as insecticides, aphicides, acaricides, and fungicides, are prepared Pesticides or aquatic organism adhesion inhibitors containing at least one of the above derivs. are claimed. Thus, 1-cyanomethyl-3-(2,6-difluorophenyl)pyrazole was stirred with NaH in THF at 50° for 30 min, followed by adding dropwise a solution of 1-(1-methyl-3,5-dichloropyrazole-4-carbonyl)pyrazole in THF at 50°, and the resulting mixture was stirred at room temperature overnight to give the title compound (I). I at 500 ppm controlled ≥80% organophosphorus-resistant Nephotettix cincticeps, Myzus persicae, larvae of Plutella xylostella Plutella xylostella konaga, and Tetranychus urticae.

IT 198072-29-6P 198072-63-8P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of ethylene derivs. as pesticides)

RN 198072-29-6 CAPLUS
CN 4-Thiazoleacetonitrile, 2-(1,1-dimethylethyl)-α-[hydroxy[4-(trifluoromethyl)-5-pyrimidinyl]methylene]- (CA INDEX NAME)



RN 198072-63-8 CAPLUS
CN Carbonic acid, 2-cyano-2-[2-(1,1-dimethylethyl)-4-thiazolyl]-1-[4-(trifluoromethyl)-5-pyrimidinyl]ethenyl methyl ester (CA INDEX NAME)

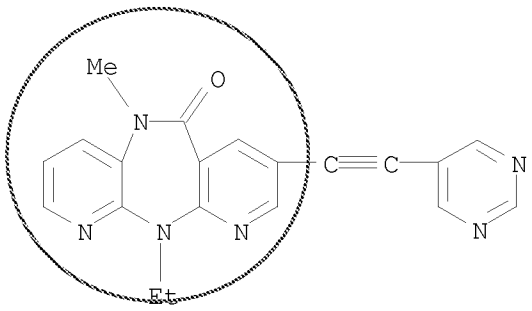


L8 ANSWER 46 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1997:350585 CAPLUS
DN 126:317394
OREF 126:61580h,61581a
TI 8-Arylalkyl- and 8-arylheteroalkyl-5,11-dihydro-6H-dipyrido[3,2-b:2',3'-e][1,4]diazepines and their use in the prevention or treatment of HIV infection
IN Cywin, Charles L.; Hoermann, Maryann; Klunder, Janice M.
PA Boehringer Ingelheim Pharmaceuticals Inc., USA
SO Eur. Pat. Appl., 62 pp.
CODEN: EPXXDW
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 767172	A1	19970409	EP 1996-115901	19961004
	EP 767172	B1	20030326		
	R: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
	CA 2187146	A1	19970407	CA 1996-2187146	19961004
	CA 2187146	C	20060103		
	JP 09188680	A	19970722	JP 1996-264860	19961004
	AT 235495	T	20030415	AT 1996-115901	19961004
	PT 767172	T	20030829	PT 1996-115901	19961004
	ES 2191075	T3	20030901	ES 1996-115901	19961004
PRAI	US 1995-4806P	P	19951006		
	US 1995-8695P	P	19951215		

OS MARPAT 126:317394
AB The invention relates to novel 8-arylalkyl-5,11-dihydro-6H-dipyrido[3,2-b:2',3'-e][1,4]diazepines of general formula I [A = (un)substituted connecting chain of 1-3 atoms, 1,2-cyclopropanediyl, oxiranediyl; Ar = certain (un)substituted (un)fused heteroarom. groups; Z = :O, :S, :NCN, :NOR8; R1 = H, alkyl, fluoroalkyl, alkenylmethyl, (hetero)aryl, alkanoyl, etc.; R2 = H, alkyl, fluoroalkyl, oxetanyl, tetrahydrofuranyl, cyano, oxazolyl, etc.; R3 = alkyl, alkenyl, alkynyl, trihalomethyl, hydroxyalkyl, halo, etc.; R4 = H, Me, halo, and R5 = H; or R3 = R5 = H, and R4 = Me or halo; or R3 = R4 = H, and R5 = alkyl, cycloalkyl, trihalomethyl, hydroxyalkyl, aryloxymethyl, etc.; or R3R4 or R4R5 forms cycloalkyl and R5 or R3 = H; or R3 = R4 = R5 = H; R6 = R7 = H; R8 = alkyl] and their pharmaceutically acceptable salts. The compds. are inhibitors of HIV-1 reverse transcriptase (RT), and are thus useful in the prevention or treatment of HIV infection. For instance, 2-chloro-5,11-dihydro-11-ethyl-8-iodo-5-methyl-6H-dipyrido[3,2-b:2',3'-e][1,4]diazepin-6-one was coupled with 4-vinylpyridine in the presence of Pd(PPh3)2Cl2 and Et3N, and the alkenylated product was reduced by aqueous Na hypophosphite in the presence of Pd black, to give title compound II. In an assay for inhibition of recombinant RT in vitro, II gave 95% inhibition at 1 mM. I were also active in a syncytial assay in human T-cells, and exhibited both high enzymic specificity for HIV-1 RT, and relatively low cytotoxicity in an MTT assay.
IT 189393-30-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of dipyridodiazepines as HIV-1 reverse transcriptase inhibitors)
RN 189393-30-4 CAPLUS

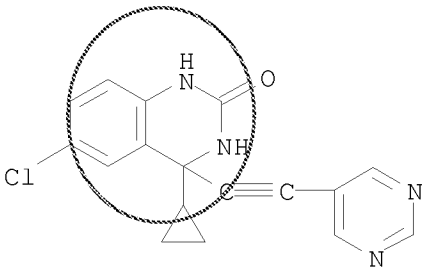
CN 6H-Dipyrido[3,2-b:2',3'-e][1,4]diazepin-6-one, 11-ethyl-5,11-dihydro-5-methyl-8-(5-pyrimidinylethynyl)- (9CI) (CA INDEX NAME)



L8 ANSWER 47 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1995:863433 CAPLUS
DN 123:256755
OREF 123:45931a,45934a
TI Preparation of 4-cyclopropyl-4-alkynylquinazolin-2-ones and related compounds as inhibitors of HIV reverse transcriptase
IN Lyle, Terry A.; Tucker, Thomas J.; Wiscount, Catherine M.
PA Merck and Co., Inc., USA
SO PCT Int. Appl., 57 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

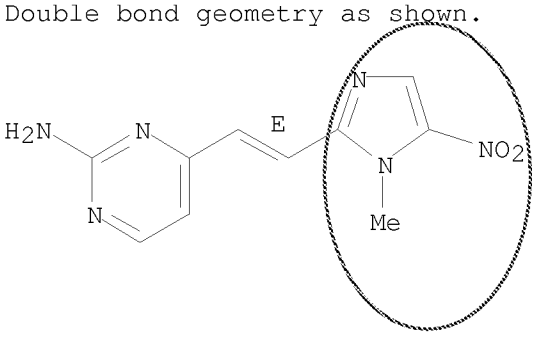
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9512583	A1	19950511	WO 1994-US12562	19941101
	W: AM, AU, BB, BG, BR, BY, CA, CN, CZ, EE, FI, GE, HU, JP, KG, KR, KZ, LK, LR, LT, LV, MD, MG, MN, NO, NZ, PL, RO, RU, SI, SK, TJ, TT, UA, UZ				
	RW: KE, MW, SD, SZ, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	AU 9510468	A	19950523	AU 1995-10468	19941101
PRAI	US 1993-148129	A	19931105		
	WO 1994-US12562	W	19941101		

OS MARPAT 123:256755
AB Title compds. [I; X = O; G = halo, NO2, cyano; n = 0-4; R1 = cycloalkyl, alkynyl, alkenyl, cyano; R2 = substituted alkenyl, alkynyl; R3 = H, cyano, amino, OH, (substituted) alkyl, alkenyl, alkynyl; R4 = H, alkyl, alkylcarbonyl, (substituted) PhCO, heterocyclylcarbonyl; with a proviso], were prepared Thus, a solution of cyclopropylmagnesium bromide in THF was treated with 5-chloroanthranilonitrile in THF at 38° and the mixture was stirred 2 h at 40° to give 64% (2-amino-4-chlorophenyl) cyclopropyl ketone. This in HOAc at 0° was treated with potassium cyanate in H2O; the mixture was stirred 1 h at 0-5° and allowed to warm to room temperature over 1 h to give 6-chloro-4-cyclopropylquinazolin-2(1H)-one. The latter in DMF was treated with NaH and then 4-methoxybenzyl chloride; the mixture was stirred 2.5 h at room temperature, 4 h at 80°, and 2.5 days at room temperature to give 6-chloro-4-cyclopropyl-1-(4-methoxybenzyl)quinazolin-2(1H)-one. This in ether was treated with magnesium triflate and then with a -78° mixture of BuLi and 2-ethynylpyridine in THF to give, after deprotection with CF3CO2H and resolution using (1S)-camphanic chloride, title compound (II). II inhibited HIV reverse transcriptase with IC50 = 7 nM. Synergistic combinations of II with AZT, ddI, etc. are claimed.
IT 153800-12-5P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 4-cyclopropyl-4-alkynylquinazolin-2-ones and related compds. as inhibitors of HIV reverse transcriptase)
RN 153800-12-5 CAPLUS
CN 2(1H)-Quinazolinone, 6-chloro-4-cyclopropyl-3,4-dihydro-4-(5-pyrimidinylethynyl)- (9CI) (CA INDEX NAME)

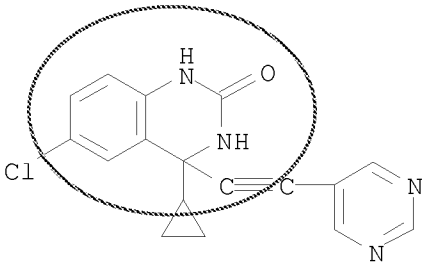

H
N
O
NH
Cl
C
C
N
N

L8 ANSWER 48 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1994:644897 CAPLUS
DN 121:244897
OREF 121:44395a,44398a
TI Qualitative organic analysis. Part 3. Identification of drugs and their metabolites by PCA of standardized TLC data
AU Romano, Guido; Caruso, Giuseppe; Musumarra, Giuseppe; Pavone, Didier; Cruciani, Gabriele
CS Istituto di Medicina Legale e delle Assicurazioni, Univ. Catania, Catania, 95124, Italy
SO Journal of Planar Chromatography--Modern TLC (1994), 7(3), 233-41
CODEN: JPCTE5; ISSN: 0933-4173
DT Journal
LA English
AB Principal components anal. (PCA) of standardized RF values of 443 drugs and their metabolites present in urine and blood samples chromatographed with four sheet systems provided a two-component model accounting for 70.8% of the total variance. The "scores" plot enabled either identification, or restriction of the range of inquiry to few candidates. This simple, cheap and fast anal. method is of vital importance in the identification of an unknown drug in cases of overdose intoxication or poisoning.
IT 62973-76-6, Azanidazole
RL: ANT (Analyte); ANST (Analytical study)
(identification of drugs and metabolites in blood and urine by principal components anal. of standardized thin-layer chromatog. data)
RN 62973-76-6 CAPLUS
CN 2-Pyrimidinamine, 4-[(1E)-2-(1-methyl-5-nitro-1H-imidazol-2-yl)ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.

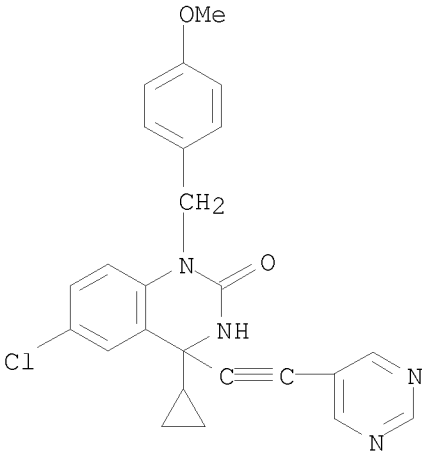


L8 ANSWER 49 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1994:534065 CAPLUS
DN 121:134065
OREF 121:24241a,24244a
TI Synthesis of a Series of 4-(Arylethynyl)-6-chloro-4-cyclopropyl-3,4-dihydroquinazolin-2(1H)-ones as Novel Non-nucleoside HIV-1 Reverse Transcriptase Inhibitors
AU Tucker, Thomas J.; Lyle, Terry A.; Wiscount, Catherine M.; Britcher, Susan F.; Young, Steven D.; Sanders, William M.; Lumma, William C.; Goldman, Mark E.; O'Brien, Julie A.; et al.
CS Merck Research Laboratories, West Point, PA, 19486, USA
SO Journal of Medicinal Chemistry (1994), 37(15), 2437-44
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
OS CASREACT 121:134065
AB As part of an ongoing effort to prepare novel non-nucleoside inhibitors of human immunodeficiency virus type-1 (HIV-1) reverse transcriptase (RT), title compds. I [R = Ph, heteroaryl, R1 = H; R = 2-pyridyl, R1 = Me] were prepared Some I were synthesized via addition of various 1-lithio-2-(aryl)alkyne nucleophiles to a 1-protected-4-cyclopropylquinazolin-2(1H)-one (II), followed by deprotection. Other I were prepared by addition of 1-lithio-2-(trimethylsilyl)acetylene to II, followed by deprotection and subsequent palladium-catalyzed coupling with various aryl halides. By incorporating an aryl group onto the end of the acetylene functionality, the requirement for a metabolically labile 3-Me group on the dihydroquinazolinone nucleus has been eliminated. A number of the target compds. were shown to be potent inhibitors of HIV-1 RT. I [R = 2-pyridyl, R1 = H], which had exhibited the most favorable overall biol. profile, was resolved via a four-step procedure. The (4S)-(-)-isomer was shown to be the active enantiomer and was selected as a candidate for further investigation.
IT 153800-12-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and HIV-1 reverse transcriptase inhibition by)
RN 153800-12-5 CAPLUS
CN 2(1H)-Quinazolinone, 6-chloro-4-cyclopropyl-3,4-dihydro-4-(5-pyrimidinylethynyl)- (9CI) (CA INDEX NAME)



IT 157195-66-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of arylethynyl(cyclopropyl)quinazolinones)
RN 157195-66-9 CAPLUS

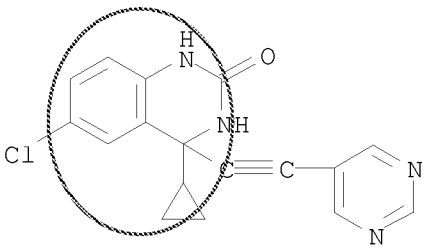
CN 2(1H)-Quinazolinone, 6-chloro-4-cyclopropyl-3,4-dihydro-1-[(4-methoxyphenyl)methyl]-4-(5-pyrimidinylethynyl)- (9CI) (CA INDEX NAME)



L8 ANSWER 50 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1994:217717 CAPLUS
DN 120:217717
OREF 120:38669a,38672a
TI Quinazoline inhibitors of HIV reverse transcriptase
IN Lyle, Terry A.; Tucker, Thomas J.; Wiscount, Catherine M.
PA Merck and Co., Inc., USA
SO Eur. Pat. Appl., 35 pp.
CODEN: EPXXDW
DT Patent
LA English
FAN.CNT 1

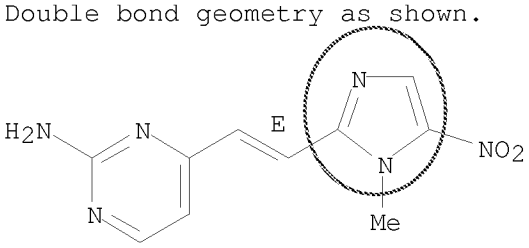
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 569083	A1	19931110	EP 1993-201232	19930429
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
	WO 9322292	A1	19931111	WO 1993-US3975	19930428
	W: AU, BB, BG, BR, CA, CZ, FI, HU, JP, KR, KZ, LK, MG, MN, MW, NO, NZ, PL, RO, RU, SD, SK, UA, US				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	AU 9342204	A	19931129	AU 1993-42204	19930428
	EP 639184	A1	19950222	EP 1993-910860	19930428
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
	HU 71401	A2	19951128	HU 1994-3187	19930428
	CA 2095194	A1	19931108	CA 1993-2095194	19930429
	AU 9338413	A	19931111	AU 1993-38413	19930506
	CN 1085550	A	19940420	CN 1993-107074	19930506
	ZA 9303179	A	19941107	ZA 1993-3179	19930506
	JP 06009578	A	19940118	JP 1993-107015	19930507
	JP 08013805	B	19960214		
	FI 9405199	A	19941104	FI 1994-5199	19941104
	NO 9404208	A	19950106	NO 1994-4208	19941104
PRAI	US 1992-880119	A	19920507		
	US 1992-991164	A	19921216		
	WO 1993-US3975	A	19930428		

OS MARPAT 120:217717
AB The title compds. I [G = halogen, NO2, CN; R1 = C3-5 cycloalkyl, C2-5 alkynyl, C2-4 alkenyl, CN; R2 = substituted C2-5 alkynyl, substituted C2-5 alkenyl; R3 = H, CN, NH2, HO, (un)substituted C1-4 alkyl, (un)substituted C2-4 alkenyl, (un)substituted C2-4 alkynyl; R4 = H, C1-4 alkyl, C1-5 alkylcarbonyl, (un)substituted benzoyl, etc.; n = 0-4], useful in the treatment of AIDS and AIDS-related complex via the inhibition of HIV reverse transcriptase, are prepared Thus, quinazoline II was prepared (m.p. 119-121°) and demonstrated 50% HIV reverse transcriptase inhibitory concentration 13 mM.
IT 153800-12-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and HIV reverse transcriptase inhibitory activity)
RN 153800-12-5 CAPLUS
CN 2(1H)-Quinazolinone, 6-chloro-4-cyclopropyl-3,4-dihydro-4-(5-pyrimidinylethynyl)- (9CI) (CA INDEX NAME)


H
N
O
NH
Cl
C
C
N
N

L8 ANSWER 51 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1992:402498 CAPLUS
DN 117:2498
OREF 117:531a,534a
TI A QSAR model of teratogenesis
AU Gombar, Vijay K.; Borgstedt, Harold H.; Enslein, Kurt; Hart, Jeffrey B.; Blake, Benjamin W.
CS Health Des., Inc., Rochester, NY, 14604, USA
SO Quantitative Structure-Activity Relationships (1991), 10(4), 306-32
CODEN: QSARDI; ISSN: 0931-8771
DT Journal
LA English
AB Four related QSAR models of teratogenesis in exptl. animals have been developed: one each for heteroarom., carboarom., alicyclic and acyclic compds. The nos. of compds. in these models range from 40 (for the alicyclic model) to 144 (for the carboarom. model). As determined by cross-validation using the leave-one-out, or jackknife, technique, the accuracy of the models in discriminating between teratogens and nonteratogens ranges from 92.4% to 96%. A single overall assessment of exptl. teratogenesis was chosen as the biol. endpoint; taking into account such factors as dosage, maternal toxicity, and affected organ systems remain to be subjects of further studies.
IT 62973-76-6, Azanidazole
RL: ADV (Adverse effect, including toxicity); PRP (Properties); BIOL (Biological study)
(teratogenesis in laboratory animals from, QSAR model of)
RN 62973-76-6 CAPLUS
CN 2-Pyrimidinamine, 4-[(1E)-2-(1-methyl-5-nitro-1H-imidazol-2-yl)ethenyl]- (CA INDEX NAME)

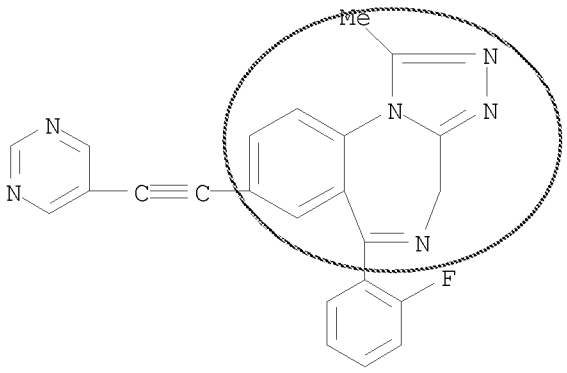
Double bond geometry as shown.



L8 ANSWER 52 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1991:143456 CAPLUS
DN 114:143456
OREF 114:24353a,24356a
TI Preparation and formulation of (heterocyclylethynyl)-triazolo[4,3-a]benzodiazepines and -thieno[3,2-f][1,2,4] triazolo [4,3-a][1,4] diazepines and analogs as platelet activating factor antagonists
IN Walser, Armin
PA Hoffmann-La Roche, Inc., USA
SO U.S., 52 pp. Cont.-in-part of U.S. Ser. No. 227,948, abandoned.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4959361	A	19900925	US 1988-252964	19881003
	ZA 8809116	A	19890830	ZA 1988-9116	19881205
	CA 1327570	C	19940308	CA 1988-585981	19881215
	DK 8807040	A	19890619	DK 1988-7040	19881216
	FI 8805820	A	19890619	FI 1988-5820	19881216
	FI 88799	B	19930331		
	FI 88799	C	19930712		
	NO 8805597	A	19890619	NO 1988-5597	19881216
	NO 167920	B	19910916		
	NO 167920	C	19911227		
	AU 8826989	A	19890629	AU 1988-26989	19881216
	AU 612441	B2	19910711		
	JP 01197484	A	19890809	JP 1988-316555	19881216
	JP 07025762	B	19950322		
	HU 50823	A2	19900328	HU 1988-6449	19881216
	HU 204273	B	19911230		
	ES 2056889	T3	19941016	ES 1988-121165	19881216
	RU 2071962	C1	19970120	RU 1988-4613119	19881216
	CN 1034722	A	19890816	CN 1988-108697	19881217
	CN 1031057	B	19960221		
	RU 2094436	C1	19971027	RU 1992-5010684	19920131
PRAI	US 1987-134726	B2	19871218		
	US 1988-227948	B2	19880803		

OS CASREACT 114:143456; MARPAT 114:143456
AB The title compds. [I; R1 = alkyl, alkoxy, CF3; R2 = H, alkyl, alkoxy, OH, AcO; R3, R4 = H, Cl, F, alkyl, alkoxy; R5 = R6(CH2)nC.tplbond.C, R7O(CH2)mC.tplbond.C; R6, R7 = aryl, heterocyclyl; X = CH:CH, S; m = 1, 2; n = 0-2; s = 0, 1] were prepared Thus, I (R1 = Me, R2 = R3 = H, R4 = 2-Cl, R5 = iodo, X = S, s = 0) was stirred 20 h with RCH2C.tplbond.CH (R = tetrahydrocarbazolo group Q) in DMF containing Et3N, CuI, Ph3P, and Pd(OAc)2 to give I (R5 = C.tplbond.CCH2Q; R1, R2, R3, R4, X, s = same as above) which had ID50 of 0.006 mg/kg orally against platelet activating factor-induced bronchoconstriction in guinea pigs.
IT 125030-55-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as platelet activating factor antagonist)
RN 125030-55-9 CAPLUS
CN 4H-[1,2,4]Triazolo[4,3-a][1,4]benzodiazepine, 6-(2-fluorophenyl)-1-methyl-8-(5-pyrimidinylethynyl)- (9CI) (CA INDEX NAME)


Me
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N
N
N
N
C
C
N
F

L8 ANSWER 53 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1990:118862 CAPLUS
DN 112:118862
OREF 112:20143a,20146a
TI Preparation and formulation of triazolodiazepine derivatives as platelet activator factor antagonists
IN Walser, Armin
PA Hoffmann-La Roche, F., und Co. A.-G., Switz.
SO Eur. Pat. Appl., 70 pp.
CODEN: EPXXDW
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 320992	A2	19890621	EP 1988-121165	19881216
	EP 320992	A3	19910109		
	EP 320992	B1	19940727		
	R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
	ZA 8809116	A	19890830	ZA 1988-9116	19881205
	CA 1327570	C	19940308	CA 1988-585981	19881215
	DK 8807040	A	19890619	DK 1988-7040	19881216
	FI 8805820	A	19890619	FI 1988-5820	19881216
	FI 88799	B	19930331		
	FI 88799	C	19930712		
	NO 8805597	A	19890619	NO 1988-5597	19881216
	NO 167920	B	19910916		
	NO 167920	C	19911227		
	AU 8826989	A	19890629	AU 1988-26989	19881216
	AU 612441	B2	19910711		
	JP 01197484	A	19890809	JP 1988-316555	19881216
	JP 07025762	B	19950322		
	HU 50823	A2	19900328	HU 1988-6449	19881216
	HU 204273	B	19911230		
	ES 2056889	T3	19941016	ES 1988-121165	19881216
	RU 2071962	C1	19970120	RU 1988-4613119	19881216
	CN 1034722	A	19890816	CN 1988-108697	19881217
	CN 1031057	B	19960221		
	RU 2094436	C1	19971027	RU 1992-5010684	19920131
PRAI	US 1987-134726	A	19871218		
	US 1988-227948	A	19880803		

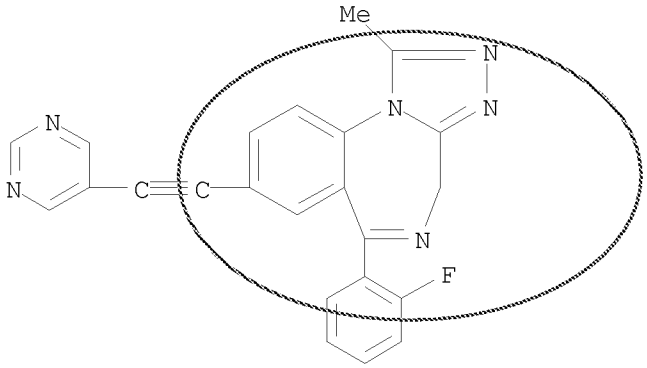
AB Title compds. [I; R1 = alkyl, alkoxy, F3C; R2 = H, alkyl, alkoxy, HO, alkanoyloxy; R3,R4 = H, Cl, F, alkyl, alkoxy; R5 = R6(CH2)nC.tplbond.C, R6,R7 = aryl, heterocyclyl; X = CH:CH, S; m = 1,2; n = 0-2; s = 0,1, with the proviso that when s = 1, R2 ≠ HO, alkoxy, alkanoyloxy; when n = 0, R6 must be attached through a C to C bond, and that R7 is always attached through a C to O bond] their enantiomers, racemates and pharmaceutically acceptable acid addition salts thereof, are prepared I are useful in diseases characterized by excess platelet activating factor (PAF) or for prevention and treatment of cardiovascular disease, pulmonary disease, immunolog. disorder, inflammatory disease, dermatol. disorders and transplant rejection. 4-(2-Chlorophenyl)-2-iodo-9-methyl-6H-thieno[3,2-f][1,2,4]triazolo[4,3-a]diazepine was reacted with 1-(2-propynyl)-1H-indazole to give I (R1 = Me; R2, R4 = H; R3 = 2-Cl; R5 = [3-(1H-indazol-1-yl)-1-propynyl]; X = S; s = 0 (II). II inhibited PAF binding to dog platelets with an IC50 of 1.0 mM and inhibited of PAF-induced bronchoconstriction in guinea pigs with an i.v. ID50 of 0.002

mg/kg. An oral suspension comprised 2-[3-[4-(2-chlorophenyl)-9-methyl-6H-thieno[3,2-f][1,2,4]triazolo[4,3-a]diazepin-2-yl]-2-propynyl]-1H-benz[de]isoquinoline-1,3(2H)-dione 5.0, hydroxypropylmethyl cellulose 8.0, polysorbate 80 0.5 g and distilled water to 100 mL.

IT 125030-55-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of triazolodiazepine platelet activating factor antagonists)

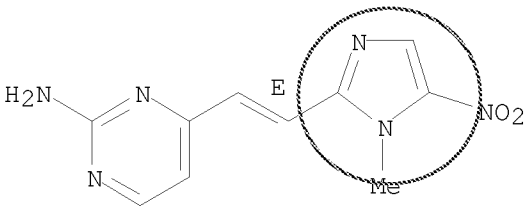
RN 125030-55-9 CAPLUS

CN 4H-[1,2,4]Triazolo[4,3-a][1,4]benzodiazepine, 6-(2-fluorophenyl)-1-methyl-8-(5-pyrimidinylethynyl)- (9CI) (CA INDEX NAME)



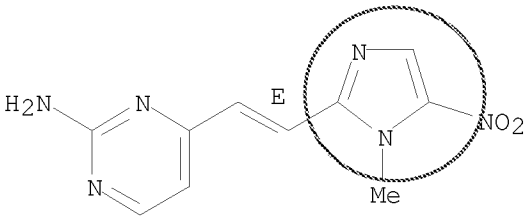
L8 ANSWER 54 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1989:566734 CAPLUS
DN 111:166734
OREF 111:27581a,27584a
TI Biliary excretion of mutagenic forms of nitroimidazoles in rats
AU Cantelli-Forti, G.; Guerra, M. C.; Scotti, M.; Hrelia, P.; Paolini, M.; Biagi, G. L.
CS Inst. Pharmacol., Univ. Bologna, Bologna, I-40126, Italy
SO Archives of Toxicology, Supplement (1989), 13(Biol. Monit. Exposure Response Subcell. Level Toxic Subst.), 333-9
CODEN: ATSUDG; ISSN: 0171-9750
DT Journal
LA English
AB The biliary excretion of 12 5-nitroimidazoles was studied in male rats and the mutagenicity of collected bile was evaluated in vitro by the Ames test with Salmonella typhimurium. Most agents were present in bile in the form of metabolites with higher mutagenicity than that of parent compds.
IT 62973-76-6, Azanidazole
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(bile excretion and mutagenicity of)
RN 62973-76-6 CAPLUS
CN 2-Pyrimidinamine, 4-[(1E)-2-(1-methyl-5-nitro-1H-imidazol-2-yl)ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.



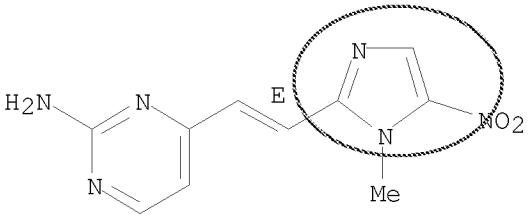
L8 ANSWER 55 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1988:31960 CAPLUS
DN 108:31960
OREF 108:5221a,5224a
TI In vivo protective role of antioxidants against genotoxicity of metronidazole and azanidazole
AU Hrelia, P.; Murelli, L.; Paolini, M.; Cantelli-Forti, G.
CS Inst. Histol. Gen. Embryol., Univ. Bologna, Bologna, 40126, Italy
SO Drugs under Experimental and Clinical Research (1987), 13(9), 577-83
CODEN: DECRDP; ISSN: 0378-6501
DT Journal
LA English
AB The mutagenicity of metronidazole and azanidazole has been extensively reported. Previous expts. demonstrated, by means of the intrasanguineous host-mediated assay, that they induced mutagenicity in liver, kidney, and lung of mice. The treatment of mice with butylated hydroxyanisole (BHA) or butylated hydroxytoluene (BHT) by 2 different routes of administration (i.p. injection and oral intubation) reduced liver- and kidney-mediated mutagenicity of azanidazole and metronidazole. No differences were observed between the routes of treatment in terms of protective effect on genotoxicity of azanidazole in the considered organs, whereas i.p. administration was the most suppressive on the mutagenicity of metronidazole. Although BHT had a protective effect against the drug-induced mutagensis, the antioxidant itself had toxic side effects in liver and lungs. The possible adverse effects on biol. systems limit the prophylactic use of BHA and BHT in preventing the action of chemical carcinogens in man.
IT 62973-76-6, Azanidazole
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(mutagenicity of, antioxidants inhibition of)
RN 62973-76-6 CAPLUS
CN 2-Pyrimidinamine, 4-[(1E)-2-(1-methyl-5-nitro-1H-imidazol-2-yl)ethenyl]-
(CA INDEX NAME)

Double bond geometry as shown.



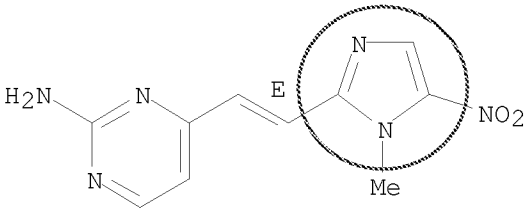
L8 ANSWER 56 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1988:217 CAPLUS
DN 108:217
OREF 108:31a,34a
TI Effects of metronidazole, azanidazole, and azathioprine on cytochrome P 450 and various mono-oxygenase activities in hepatic microsomes from control and induced mice
AU Cantelli-Forti, G.; Paolini, M.; Hrelia, P.; Sapigni, E.; Biagi, G. L.
CS Ist. Farmacol., Univ. Bologna, Bologna, 48-40126, Italy
SO Archives of Toxicology, Supplement (1987), Volume Date 1986, 11(Mech. Models Toxicol.), 264-9
CODEN: ATSUDG; ISSN: 0171-9750
DT Journal
LA English
AB Imidazole-related drugs may affect the metabolism of other chemical Thus, pharmacokinetic interactions may be a consequence of the coadministration of metronidazole, azanidazole, and azathioprine with other drugs which are biotransformed by the mixed-function oxidase system. The effects of these imidazole drugs on various monooxygenase enzymes are presented.
IT 62973-76-6, Azanidazole
RL: BIOL (Biological study)
(monooxygenase of liver microsome response to, drug interaction in relation to)
RN 62973-76-6 CAPLUS
CN 2-Pyrimidinamine, 4-[(1E)-2-(1-methyl-5-nitro-1H-imidazol-2-yl)ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.



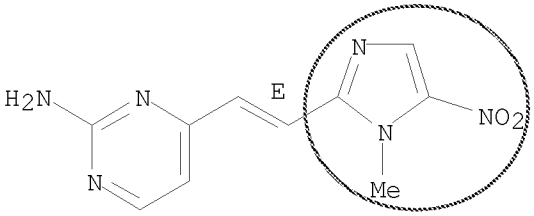
L8 ANSWER 57 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1987:43364 CAPLUS
DN 106:43364
OREF 106:7053a,7056a
TI The influence of physicochemical parameters on the biliary excretion of a series of nitroimidazoles
AU Biagi, Gian Luigi; Cantelli-Forti, Giorgio; Barbaro, Anna Maria; Guerra, Maria Clelia; Hrelia, Patrizia; Borea, Pier Andrea
CS Ist. Farmacol., Univ. Bologna, Bologna, Italy
SO Journal of Medicinal Chemistry (1987), 30(2), 420-3
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
AB The relationship between the physicochem. parameters and biliary excretion of 12 nitroimidazoles (I; R1 = H, Me, hydroxyethyl, 2-(morpholinyl)ethyl, CH2CH2SO2Et, etc.; R2 = H, Me, CHO, iso-Pr, CH2OH, etc.), which are antibacterial, antitrichomonal, and antiamebic agents, was investigated. Reverse-parabolic relationship was shown between the Rm (a hydrophobicity constant) values and the biliary excretion of the test compds. In other words, the compds. closer to the optimal Rm value are excreted less than those characterized by higher or lower Rm values. Since the Rm values seem to account for both the lipophilic and polar character of nitroimidazoles, the reversed parabola could be due to plasma protein binding and(or) some protein binding within the hepatocyte. In fact, both the lipophilic and polar character seem to play an important role in protein binding of chems.
IT 62973-76-6, Azanidazole
RL: PROC (Process)
(excretion of, in bile, physicochem. parameters in)
RN 62973-76-6 CAPLUS
CN 2-Pyrimidinamine, 4-[(1E)-2-(1-methyl-5-nitro-1H-imidazol-2-yl)ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.



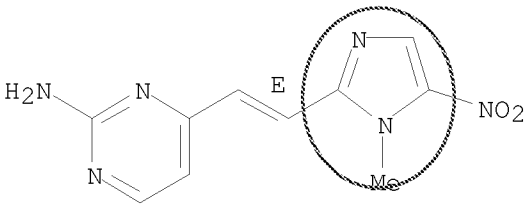
L8 ANSWER 58 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1986:141778 CAPLUS
DN 104:141778
OREF 104:22227a,22230a
TI The organospecific activity of metronidazole and azanidazole in the intrasanguineous host-mediated assay
AU Cantelli-Forti, G.; Hrelia, P.; Paolini, M.; Bronzetti, G.; Biagi, G. L.
CS Inst. Pharmacol., Univ. Bologna, Bologna, Italy
SO Drugs under Experimental and Clinical Research (1985), 11(11), 755-9
CODEN: DECRDP; ISSN: 0378-6501
DT Journal
LA English
AB The genotoxicity of nitroimidazoles and in particular their potential carcinogenicity has been demonstrated. In order to investigate the specific target organ(s) for these drugs or their metabolites, a method for measuring mutations in microorganisms, with reference to the metabolism of mammals, was used in mice. Metronidazole (I) [443-48-1] and azanidazole (II) [62973-76-6] were tested for their ability to induce genetic effects in a diploid strain (D7) of Saccharomyces cerevisiae in the intrasanguineous host-mediated assay. The test compds. showed dose-related increases of point mutation and mitotic gene conversion frequencies in liver, kidney and lung. Azanidazole seemed to favor the kidney and the liver although increases in genotoxicity were observed also in the lung. Metronidazole was toxic and induced both point mutation and mitotic gene conversion when recovered from the liver. Yeast recovered from the kidney and the lung showed an increase especially in point mutation. The mechanisms involved in the mutagenicity of nitroimidazoles are discussed.
IT 62973-76-6
RL: PRP (Properties)
(genotoxicity of, organ specificity in and assay for evaluation of)
RN 62973-76-6 CAPLUS
CN 2-Pyrimidinamine, 4-[(1E)-2-(1-methyl-5-nitro-1H-imidazol-2-yl)ethenyl]-
(CA INDEX NAME)

Double bond geometry as shown.



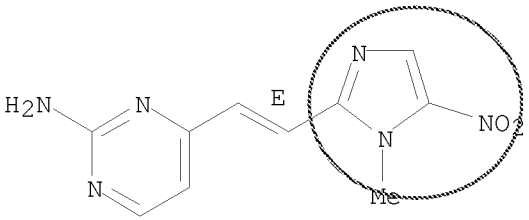
L8 ANSWER 59 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1986:122576 CAPLUS
DN 104:122576
OREF 104:19191a,19194a
TI Relationship between lipophilic character and urinary excretion of nitroimidazoles and nitrothiazoles in rats
AU Cantelli Forti, Giorgio; Guerra, Maria Clelia; Barbaro, Anna Maria; Hrelia, Patrizia; Biagi, Gian Luigi; Borea, Pier Andrea
CS Ist. Farmacol., Univ. Bologna, Bologna, Italy
SO Journal of Medicinal Chemistry (1986), 29(4), 555-61
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
AB QSAR (lipophilicity) for the urinary excretion (in rats) of 26 title compds. {I; R1 = H, Me, 2-hydroxyethyl, 4-diethylaminoethyl-2-oxyethyl, 2,3-dihydroxypropyl, 2-(4-methyl-1,4-dihydropyrazin-1-yl)ethyl, 2-morpidinoethyl, etc.; R3 = H, Me iso-Pr, cyclopropyl, 2-carboxy-2phenoxyethenyl, 2-(2-amino-4-pyrimidinyl)ethenyl, 2-(2-benzodioxalan-5-yl)ethenyl, etc.; X = N or S}, which are used for the treatment of urinary tract infections and no radiosensitizers, was studied. The urinary excretion of unmetabolized I was parabolically related with log P, an expression of lipophilicity.
IT 62973-76-6
RL: PROC (Process)
(excretion of, in urine, QSAR in)
RN 62973-76-6 CAPLUS
CN 2-Pyrimidinamine, 4-[(1E)-2-(1-methyl-5-nitro-1H-imidazol-2-yl)ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.

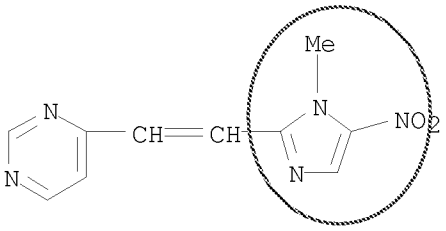


L8 ANSWER 60 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1986:95558 CAPLUS
DN 104:95558
OREF 104:15045a,15048a
TI Qualitative organic analysis. I. Identification of drugs by principal components analysis of standardized thin-layer chromatographic data in four eluent systems
AU Musumarra, Giuseppe; Scarlata, Giuseppe; Cirma, Giuseppe; Romano, Guido; Palazzo, Silvana; Clementi, Sergio; Giulietti, Gianfranco
CS Dip. Sci. Chim., Univ. Catania, Catania, 95125, Italy
SO Journal of Chromatography (1985), 350(1), 151-68
CODEN: JOCRAM; ISSN: 0021-9673
DT Journal
LA English
AB Identification of drugs by principal component anal. of standardized retention factor (RF) values in 4 eluent systems, [EtOAc [141-78-6]-MeOH [67-56-1]-30% NH4OH (85:10:15), cyclohexane [110-82-7]-PhMe [108-88-3]-Et2NH [109-89-7] (65:25:10), EtOAc-CHCl3 [67-66-3] (50:50), and Me2CO [67-64-1] with the plate dipped in KOH solution] provided a 2-component model which accounts for 73% of the total variance. The scores plot allowed the restriction of the range of inquiry to a few candidates. This result is of great practical significance in anal. toxicol., especially when account is taken of the cost, the time, the anal. instrumentation and the simplicity of the calcns. required by the method.
IT 62973-76-6
RL: ANT (Analyte); ANST (Analytical study)
(identification of, by TLC in four eluent systems)
RN 62973-76-6 CAPLUS
CN 2-Pyrimidinamine, 4-[(1E)-2-(1-methyl-5-nitro-1H-imidazol-2-yl)ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.

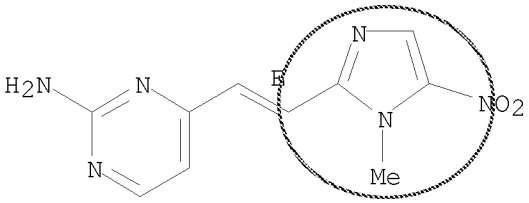


L8 ANSWER 61 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1984:603875 CAPLUS
DN 101:203875
OREF 101:30726h,30727a
TI Nitroimidazoles: part XIX - structure-activity relationships
AU Nagarajan, K.; Arya, V. P.; George, T.; Nair, M. D.; Sudarsanam, V.; Ray, D. K.; Shrivastava, V. B.
CS Res. Cent., CIBA-GEIGY, Bombay, 400 063, India
SO Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1984), 23B(4), 342-62
CODEN: IJSBDB; ISSN: 0376-4699
DT Journal
LA English
AB A variety of nitroimidazoles, mostly 1,2-disubstituted-5-nitro derivs. were examined for in vitro activity against Entamoeba histolytica and for effectiveness in treating early hepatic infection in golden hamsters. Many compds. carried a functionalized N atom at position 2. In vivo activity was observed with 1-alkyl-5-nitroimidazoles carrying a substituted imidazolidinone or imidazole. Among these derivs., 1-methylsulfonyl-3-(1-methyl-5-nitro-2-imidazolyl)-2-imidazolidinone (I) [56302-13-7] was the most potent against hepatic and caecal infections of E. histolytica in the golden hamster and Trichomonas foetus infections in mice. It was developed as a drug for treatment of amoebiasis, giardiasis, and trichomoniasis. The structure-antiamebic activity relationships of the nitroimidazoles are discussed.
IT 87008-24-0
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(amebicidal activity of, structure in relation to)
RN 87008-24-0 CAPLUS
CN Pyrimidine, 4-[2-(1-methyl-5-nitro-1H-imidazol-2-yl)ethenyl]- (CA INDEX NAME)



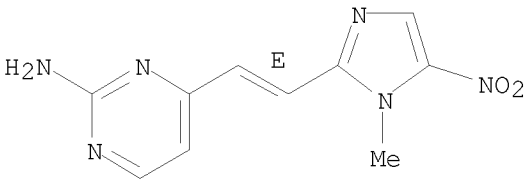
L8 ANSWER 62 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1984:563253 CAPLUS
DN 101:163253
OREF 101:24535a,24538a
TI Urinary excretion of mutagenic forms of metronidazole and nine related compounds as detected by HPLC
AU Cantelli Forti, G.; Guerra, M. C.; Hrelia, P.; Barbaro, A. M.; Biagi, G. L.
CS Inst. Pharmacol., Univ. Bologna, Bologna, Italy
SO Drugs under Experimental and Clinical Research (1984), 10(5), 325-31
CODEN: DECRDP; ISSN: 0378-6501
DT Journal
LA English
AB Metabolites of a series of 10 5-nitroimidazoles (I; R1 = Me, (CH)2OH, N-alkylpyrimidamine, etc. R2 = Me, CHO, CH2CO2NH2, p-allylpyrimidamine, etc.) were identified and their mutagenic activity in rat urine evaluated by the Ames test. At least 3 I are biotransformed into active metabolites which increased the overall mutagenic activity in urine. Metronidazole [443-48-1], despite a 157% increase in mutagenicity on biotransformation, seems to be the compound with the lowest risk potential.
IT 62973-76-6D, metabolites
RL: FORM (Formation, nonpreparative)
(formation of, mutagenicity in relation to)
RN 62973-76-6 CAPLUS
CN 2-Pyrimidinamine, 4-[(1E)-2-(1-methyl-5-nitro-1H-imidazol-2-yl)ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.



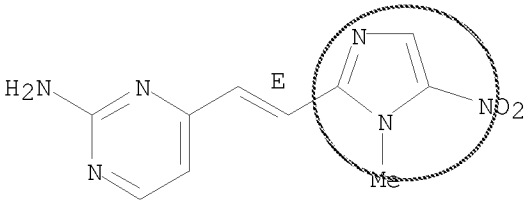
IT 62973-76-6
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(mutagenicity of, metabolism in relation to)
RN 62973-76-6 CAPLUS
CN 2-Pyrimidinamine, 4-[(1E)-2-(1-methyl-5-nitro-1H-imidazol-2-yl)ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.



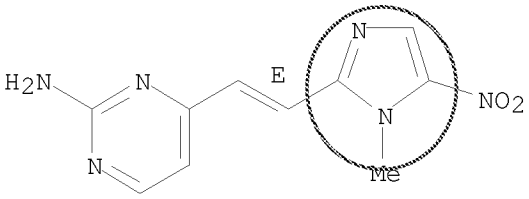
L8 ANSWER 63 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1984:153742 CAPLUS
DN 100:153742
OREF 100:23381a,23384a
TI Electroreduction, mutagenicity and antimicrobial activity of 5-nitroimidazole derivatives
AU Aicardi, G.; Cantelli Forti, G.; Guerra, M. C.; Barbaro, A. M.; Biagi, G. L.
CS Ist. Farmacol., Univ. Bologna, Bologna, Italy
SO Developments in Oncology (1983), 15(Control Tumour Growth Its Biol. Bases), 300-8
CODEN: DEOND5; ISSN: 0167-4927
DT Journal
LA English
AB When 25 nitroimidazoles and 2 nitrothiazoles were tested in vitro, a close pos. correlation was found between the relative potencies in the mutagenic and antibacterial assays, suggesting that the 2 activities occur via the same mechanism. The electroredn. potentials (ERP) at pH 7.4 ranged from -790 to -410 mV. Compds. having the highest mutagenic activity, i.e., azanidazole, niridazole, and DA 3832 had the least neg. ERP values. This indicated that all active compds. must be reducible and that a significant correlation should exist between ERP and mutagenic activity.
IT 62973-76-6
RL: PRP (Properties)
(antimicrobial activity and mutagenicity and electroredn. potential of, structure in relation to)
RN 62973-76-6 CAPLUS
CN 2-Pyrimidinamine, 4-[(1E)-2-(1-methyl-5-nitro-1H-imidazol-2-yl)ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.



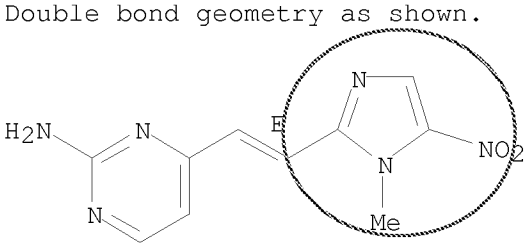
L8 ANSWER 64 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1984:99758 CAPLUS
DN 100:99758
OREF 100:15097a,15100a
TI Electroreduction, mutagenicity and antimicrobial activity of 5-nitroimidazole derivatives
AU Aicardi, G.; Cantelli Forti, G.; Guerra, M. C.; Barbaro, A. M.; Biagi, G. L.
CS Ist. Farmacol., Univ. Bologna, Bologna, Italy
SO Fortschritte der Onkologie (1983), 10(Control Tumour Growth Its Biol. Bases), 300-8
CODEN: FONKDF; ISSN: 0323-5084
DT Journal
LA English
AB A series of 25 nitroimidazoles and 2 nitrothiazole derivs. were tested for their mutagenic and antibacterial activities. The relative potencies in the mutagenic (Ames/Salmonella test) and antibacterial (cylinder-plate method) assays showed a close correlation, supporting the hypothesis that the 2 activities occur via the same mechanism. The electroredn. potentials of the 27 compds. at pH 7.4 ranged between -790 and -410 mV. The compds. most active in the mutagenic assay, i.e., azanidazole, niridazole, and DA-3832, had the least neg. electroredn. values. Structure-activity relations are discussed.
IT 62973-76-6
RL: BIOL (Biological study)
(antibacterial and mutagenic activity of, structure in relation to)
RN 62973-76-6 CAPLUS
CN 2-Pyrimidinamine, 4-[(1E)-2-(1-methyl-5-nitro-1H-imidazol-2-yl)ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.

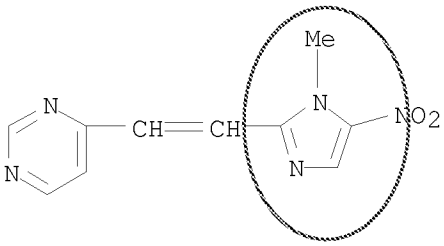


L8 ANSWER 65 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1984:63245 CAPLUS
DN 100:63245
OREF 100:9569a,9572a
TI Quantitative relationship between structure and mutagenic activity in series of 5-nitroimidazoles
AU Biagi, G. L.; Barbaro, A. M.; Guerra, M. C.; Cantelli Forti, G.; Aicardi, G.; Borea, P. A.
CS Ist. Farmacol., Univ. Bologna, Bologna, Italy
SO Teratogenesis, Carcinogenesis, and Mutagenesis (1983), 3(5), 429-38
CODEN: TCMUD8; ISSN: 0270-3211
DT Journal
LA English
AB The mutagenic activity of 20 5-nitroimidazoles (I) was tested in Salmonella typhimurium TA 100 strain by means of the Ames test. A multiple regression anal. using the interaction term molar refractivity (MR2) + H bonding (Hb) and the chromatog. Rm values yielded the equation: log 1/C = 3.805 + 0.680 MR2 + Hb + 0.548 Rm - 0.749 Rm2 (r = 0.926, F = 32.205) where C is the molar concentration (1 + 10-6 M) of each drug increasing the revertants by 5 times in the Ames test. The interaction term MR2 + Hb takes into account the pos. effect exerted by substituents characterized by higher MR2 and capable of Hb. When the electroredn. potentials were included, the correlation was not improved.
IT 62973-76-6
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(mutagenicity of, structure in relation to)
RN 62973-76-6 CAPLUS
CN 2-Pyrimidinamine, 4-[(1E)-2-(1-methyl-5-nitro-1H-imidazol-2-yl)ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.

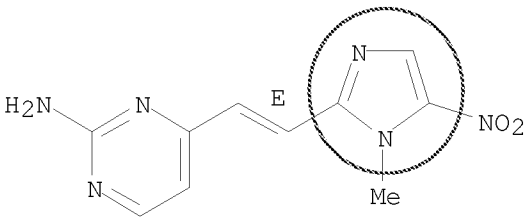


L8 ANSWER 66 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1983:522370 CAPLUS
DN 99:122370
OREF 99:18849a,18852a
TI Nitroimidazoles: Part XV. 1-Methyl-5-nitro-2-oxy(mercapto)imidazoles, 1-methyl-5-nitroimidazole-2-methanol (carboxaldehyde and glyoxalic ester) derivatives and 1-substituted alkyl-2-methyl-5- and -4-nitroimidazoles
AU Arya, V. P.; Nagarajan, K.; Shenoy, S. J.
CS Ciba-Geigy Res. Cent., Bombay, 400 063, India
SO Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1982), 21B(12), 1078-86
CODEN: IJSBDB; ISSN: 0376-4699
DT Journal
LA English
AB Approx. 60 title imidazoles were prepared by standard reactions. Thus, displacement reactions on I (R = MeSO2) with phenols gave I (R = p-OCHC6H4, 1-oxido-3-pyridyl).
IT 87008-24-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 87008-24-0 CAPLUS
CN Pyrimidine, 4-[2-(1-methyl-5-nitro-1H-imidazol-2-yl)ethenyl]- (CA INDEX NAME)



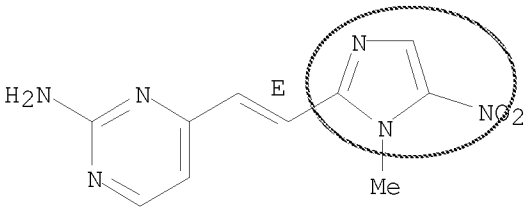
L8 ANSWER 67 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1983:410764 CAPLUS
DN 99:10764
OREF 99:1705a,1708a
TI RM values, retention times and octanol-water partition coefficients of a series of 5-nitroimidazoles
AU Guerra, M. C.; Barbaro, A. M.; Cantelli Forti, G.; Biagi, G. L.; Borea, P. A.
CS Ist. Farmacol., Univ. Bologna, Bologna, Italy
SO Journal of Chromatography (1983), 259(2), 329-33
CODEN: JOCRAM; ISSN: 0021-9673
DT Journal
LA English
AB The partition coeffs. of I derivs. in octanol-water were evaluated by high-performance liquid chromatog. on a μBondapak C18 column with MeOH-H2O (2:3) at 1 mL/min, and retention times were expressed as log capacity factor (k') and compared relative retention times (RM). For the 22 I studied, log k' values were better correlated with log partition coeffs. than were RM values, even if the latter were corrected for stationary phase binding.
IT 62973-76-6
RL: PRP (Properties)
(partition coefficient of, in octanol-water, high-performance liquid chromatog. in)
RN 62973-76-6 CAPLUS
CN 2-Pyrimidinamine, 4-[(1E)-2-(1-methyl-5-nitro-1H-imidazol-2-yl)ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.



L8 ANSWER 68 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1983:122094 CAPLUS
DN 98:122094
OREF 98:18557a,18560a
TI Mutagenicity of a series of 25 nitroimidazoles and two nitrothiazoles in Salmonella typhimurium
AU Cantelli-Forti, G.; Aicardi, G.; Guerra, M. C.; Barbaro, A. M.; Biagi, G. L.
CS Ist. Farmacol., Univ. Stud. Bologna, Bologna, Italy
SO Teratogenesis, Carcinogenesis, and Mutagenesis (1983), 3(1), 51-63
CODEN: TCMUD8; ISSN: 0270-3211
DT Journal
LA English
AB The mutagenicity and antibacterial action of the title radiosensitizers were examined in S. typhimurium. For 22 of the compds., the number of revertants increased with drug concentration, reaching a peak and then falling out. The falling out of the mutagenic activity appeared to be related to antibacterial activity as the 5 compds. that had no mutagenic effect also exhibited no antibacterial activity. The curve for the relation between mutagenicity and antibacterial activity had a slope close to 1.
IT 62973-76-6
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(mutagenicity of, in Salmonella typhimurium, antibacterial activity in relation to)
RN 62973-76-6 CAPLUS
CN 2-Pyrimidinamine, 4-[(1E)-2-(1-methyl-5-nitro-1H-imidazol-2-yl)ethenyl]- (CA INDEX NAME)

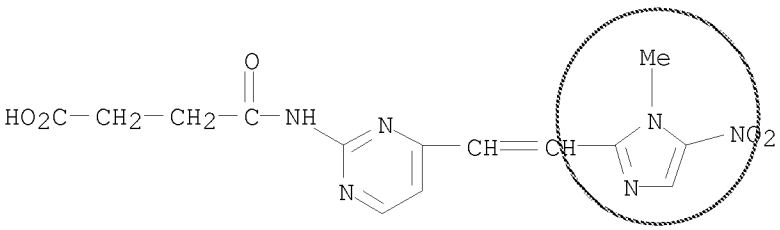
Double bond geometry as shown.



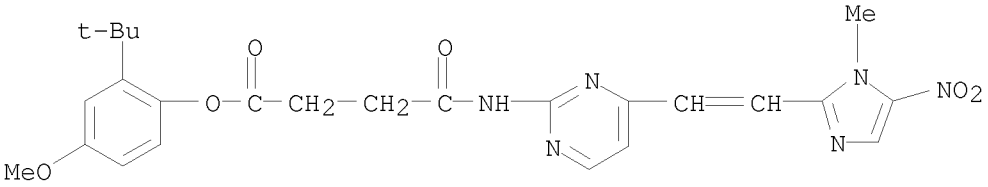
L8 ANSWER 69 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1982:162735 CAPLUS
DN 96:162735
OREF 96:26795a,26798a
TI Antibacterial and antiprotozoan derivatives and compositions containing them
PA Farmatis S.r.l., Italy
SO Belg., 17 pp.
CODEN: BEXXAL
DT Patent
LA French
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	BE 889875	A1	19811201	BE 1981-205595	19810806
	GB 2081706	A	19820224	GB 1980-25832	19800807
	GB 2081706	B	19840307		
	EP 45990	A1	19820217	EP 1981-200869	19810803
	R: AT, DE, GB, NL, SE				
	ES 504585	A1	19820601	ES 1981-504585	19810806
	FR 2488256	A1	19820212	FR 1981-15327	19810807
	FR 2488256	B1	19831118		
PRAI	GB 1980-25832	A	19800807		

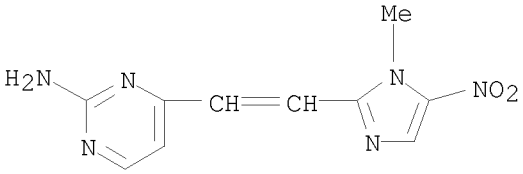
OS MARPAT 96:162735
AB The esters I (R = alkyl; R1 = H, OMe) were prepared Thus azanidazole was acylated with succinic anhydride and esterified with 4,2-MeO(Me3C)C6H3OH to give I (R = Me, R1 = OMe).
IT 81403-87-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and esterification of)
RN 81403-87-4 CAPLUS
CN Butanoic acid, 4-[[4-[2-(1-methyl-5-nitro-1H-imidazol-2-yl)ethenyl]-2-pyrimidinyl]amino]-4-oxo- (CA INDEX NAME)



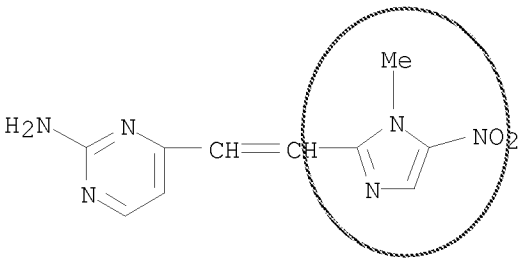
IT 81403-88-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 81403-88-5 CAPLUS
CN Butanoic acid, 4-[[4-[2-(1-methyl-5-nitro-1H-imidazol-2-yl)ethenyl]-2-pyrimidinyl]amino]-4-oxo-, 2-(1,1-dimethylethyl)-4-methoxyphenyl ester (CA INDEX NAME)



IT 53409-75-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with succinic anhydride)
RN 53409-75-9 CAPLUS
CN 2-Pyrimidinamine, 4-[2-(1-methyl-5-nitro-1H-imidazol-2-yl)ethenyl]- (CA INDEX NAME)

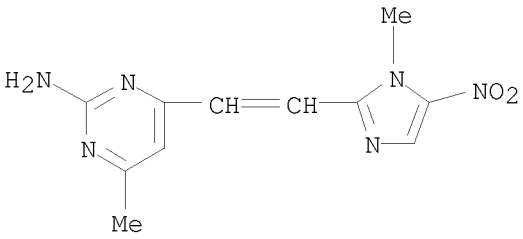


L8 ANSWER 70 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1982:103385 CAPLUS
DN 96:103385
OREF 96:16965a,16968a
TI Utilization of deuterium labeling and carbon-13 NMR spectroscopy in the investigation of the condensation of 1-methyl-5-nitroimidazole-2-aldehyde and 2-amino-4-methylpyrimidine
AU Bradamante, Silvia; Colombo, Silvana; Vittadini, Giorgio
CS Ist. Chim. Ind., Univ. Milan, Milan, 20133, Italy
SO Journal of Heterocyclic Chemistry (1981), 18(7), 1399-403
CODEN: JHTCAD; ISSN: 0022-152X
DT Journal
LA English
AB The condensation of I with II in HOAc-H2SO4 to give III (R = H); the condensation did not occur in the absence of H2SO4. This, the formation of III (R = D), partially deuterated in the NH2 group and at C-5, from the condensation reaction with II-Me-d3, and the H-D exchange in II indicate that the O-protonated I.H+ and IV are the active condensation reaction intermediates. The 1H and 13C NMR of I or II in DMSO, CF3CO2H, HOAc, or HOAc-H2SO4 support this mechanism. The 13C and 1H NMR of partially deuterated III (R = D) are used to assign the NMR of III (R = H).
IT 81009-16-7 81009-17-8
RL: PRP (Properties)
(carbon-13 and proton NMR of)
RN 81009-16-7 CAPLUS
CN 2-Pyrimidinamine, 4-[2-(1-methyl-5-nitro-1H-imidazol-2-yl)ethenyl]-, conjugate monoacid (9CI) (CA INDEX NAME)

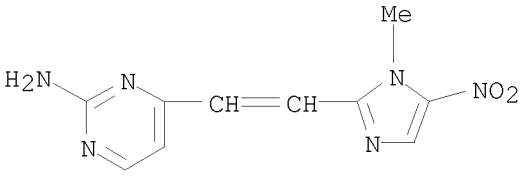


● H^+

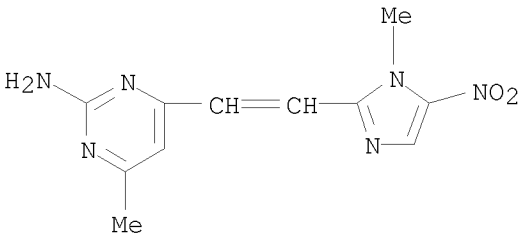
RN 81009-17-8 CAPLUS
CN 2-Pyrimidinamine, 4-methyl-6-[2-(1-methyl-5-nitro-1H-imidazol-2-yl)ethenyl]-, conjugate monoacid (9CI) (CA INDEX NAME)



IT 53409-75-9P 81009-14-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and carbon-13 and proton NMR of)
RN 53409-75-9 CAPLUS
CN 2-Pyrimidinamine, 4-[2-(1-methyl-5-nitro-1H-imidazol-2-yl)ethenyl]- (CA INDEX NAME)

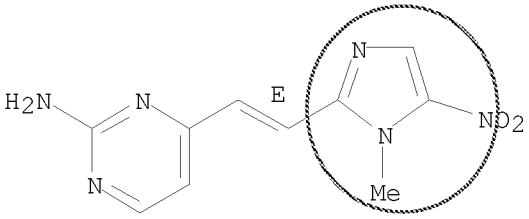


RN 81009-14-5 CAPLUS
CN 2-Pyrimidinamine, 4-methyl-6-[2-(1-methyl-5-nitro-1H-imidazol-2-yl)ethenyl]- (CA INDEX NAME)



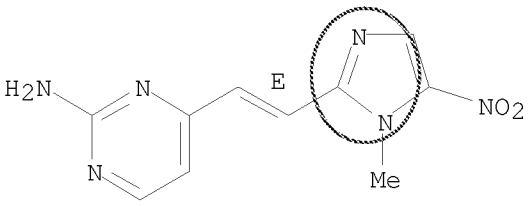
L8 ANSWER 71 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1982:29702 CAPLUS
DN 96:29702
OREF 96:4845a,4848a
TI RM and log P values of 5-nitroimidazoles
AU Guerra, M. C.; Barbaro, A. M.; Cantelli Forti, G.; Foffani, M. T.; Biagi, G. L.; Borea, P. A.; Fini, A.
CS Ist. Farmacol., Univ. Bologna, Bologna, Italy
SO Journal of Chromatography (1981), 216, 93-102
CODEN: JOCRAM; ISSN: 0021-9673
DT Journal
LA English
AB The chromatog. RM values of a series of nitroimidazoles and their log P values were determined in view of a study of their structure-activity relations as mutagenic agents. The equations describing the relation between RM and log P values show a low correlation coefficient The introduction of the molar refractivity of the R1 and R2 groups yields a significant improvement in the correlation coefficient The molar refractivity could be an expression of the adsorption activity of the silica gel layer.
IT 62973-76-6
RL: BIOL (Biological study)
(chromatog. and log P values of, mutagenicity in relation to)
RN 62973-76-6 CAPLUS
CN 2-Pyrimidinamine, 4-[(1E)-2-(1-methyl-5-nitro-1H-imidazol-2-yl)ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.



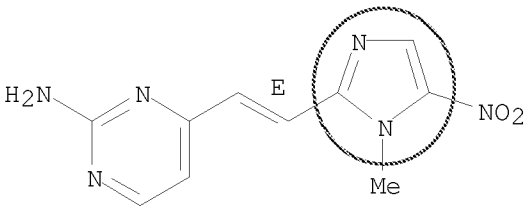
L8 ANSWER 72 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1980:174123 CAPLUS
DN 92:174123
OREF 92:28063a,28066a
TI High-performance liquid chromatographic determination of the nitroimidazole azanidazole in human plasma and urine
AU Brodie, R. R.; Chasseaud, L. F.; Walmsley, L. M.; Darragh, A.; O'Kelly, D. A.
CS Dep. Metab. Pharmacokinet., Huntingdon Res. Cent., Huntingdon, UK
SO Journal of Chromatography (1979), 179(2), 301-9
CODEN: JOCRAM; ISSN: 0021-9673
DT Journal
LA English
AB Peak mean plasma concns. of azanidazole (I) [62973-76-6] of 267 ng/mL occurred 1.5 h after single oral doses to human subjects and declined with a half-life of 0.8 h. Less than 0.5% of the dose was excreted in the urine as unchanged drug. Metabolites of I were detected but not pos. identified. A reversed-phase high-performance chromatog. method using UV detection is presented for the determination of I.
IT 62973-76-6
RL: ANT (Analyte); ANST (Analytical study)
(determination of, in blood and urine , pharmacokinetics in relation to)
RN 62973-76-6 CAPLUS
CN 2-Pyrimidinamine, 4-[(1E)-2-(1-methyl-5-nitro-1H-imidazol-2-yl)ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.



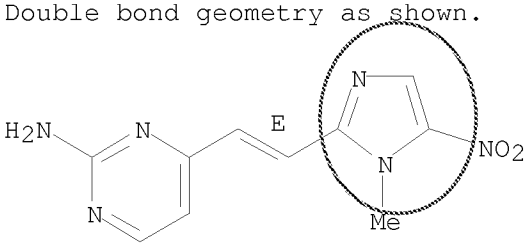
L8 ANSWER 73 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1979:115134 CAPLUS
DN 90:115134
OREF 90:18067a,18070a
TI Toxicological and teratological studies of azanidazole
AU Tammiso, R.; Olivari, G.; Coccoli, C.; Garzia, G.; Vittadini, G.
CS Res. Cent., Ist. Chemioter. Italiano, Milan, Italy
SO Arzneimittel-Forschung (1978), 28(12), 2251-6
CODEN: ARZNAD; ISSN: 0004-4172
DT Journal
LA English
AB Azanidazole (I) [62973-76-6] was well tolerated by rats and rabbits when administered as a single dose or repeated daily doses for 6 mo. Furthermore, no adverse reproductive effects and no evidence of teratogenic activity were observed in all of the tested animals. Survival indexes were not affected, and body weight of progeny was normal in all studies on reproduction and peri- and post-natal toxicity.
IT 62973-76-6P
RL: PREP (Preparation)
(reproduction and teratogenesis response to)
RN 62973-76-6 CAPLUS
CN 2-Pyrimidinamine, 4-[(1E)-2-(1-methyl-5-nitro-1H-imidazol-2-yl)ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.



L8 ANSWER 74 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1978:522766 CAPLUS
DN 89:122766
OREF 89:18867a,18870a
TI Azanidazole
AU De Angelis, L.
CS Italy
SO Drugs of Today (1978), 14(6), 232-6
CODEN: MDACAP; ISSN: 0025-7656
DT Journal; General Review
LA English/Spanish
AB A review with 7 refs. on azanidazole (I) [62973-76-6].
IT 62973-76-6
RL: BIOL (Biological study))
RN 62973-76-6 CAPLUS
CN 2-Pyrimidinamine, 4-[(1E)-2-(1-methyl-5-nitro-1H-imidazol-2-yl)ethenyl]-
(CA INDEX NAME)

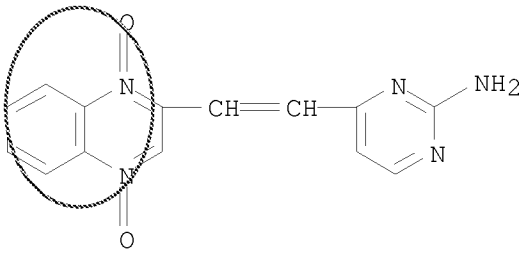
Double bond geometry as shown.



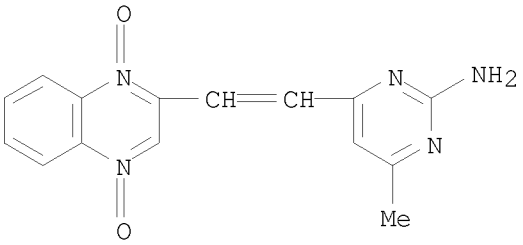
L8 ANSWER 75 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1978:506419 CAPLUS
DN 89:106419
OREF 89:16371a,16374a
TI Promoting the growth and improving the feed utilization of animals
IN Ivy, Richard E.; Williams, Robert D.
PA IMC Chemical Group, Inc., USA
SO Ger. Offen., 24 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2755063	A1	19780622	DE 1977-2755063	19771208
	DE 2755063	C2	19891214		
	US 4128642	A	19781205	US 1976-752596	19761220
	CA 1105765	A1	19810728	CA 1977-291249	19771118
	GB 1554985	A	19791031	GB 1977-48423	19771121
	JP 53081386	A	19780718	JP 1977-151843	19771219
	JP 61027027	B	19860623		
	FR 2374321	A1	19780713	FR 1977-38452	19771220
	FR 2374321	B1	19820528		
PRAI	US 1976-752596	A	19761220		

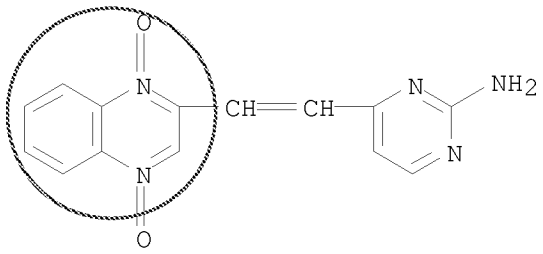
OS MARPAT 89:106419
AB Substituted quinoxaline dioxides I (R = H, Me, Et, n-Pr, iso-Pr, n-Bu, iso-Bu, or 1-methylpropyl are prepared and used for promoting growth and improving feed utilization by livestock. The I leave low toxicity and are orally administered at 10-150 g/ton of feed. I are prepared by treating quinoxaline di-N-oxide-2-carboxyaldehyde dimethylacetate (II) [32065-66-0] or its derivs. with a substituted pyrimidine in an organic solvent, e.g., AcOH in the presence of a strong acid such as concentrated H2SO4 for 10-24 h at 25-50° or higher temperature For example, a mixture of 15 mL 99% HCO2H, 1.15 g 96% H2SO4, 1.09 g (0.01 mol) 2-amino-4-methylpyrimidine [108-52-1] and 2.36 g (0.01 mol) II was heated at 45-50° for 10 h then cooled and diluted with 35 mL cold H2O. On adjusting the pH to .apprx.5 with NaHCO3, a yellow precipitate was formed which was filtered and washed. The resulting product was 2-[2-(2-amino-4-pyrimidinyl)-ethenyl]-quinoxaline 1,4-dioxide (III) [59985-27-2], m.p. 237-9° (decomposed) yielding 1.8 g (64%) III. Chickens were fed a mixed feed containing 100 g III/ton, and after 28 days average weight increased
3.1% and feed efficiency improved 2.8% more than in control groups.
IT 59985-27-2P 65268-96-4P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as animal growth stimulant)
RN 59985-27-2 CAPLUS
CN 2-Pyrimidinamine, 4-[2-(1,4-dioxido-2-quinoxalinyl)ethenyl]- (CA INDEX NAME)



RN 65268-96-4 CAPLUS
CN 2-Pyrimidinamine, 4-[2-(1,4-dioxido-2-quinoxalinyl)ethenyl]-6-methyl- (CA INDEX NAME)



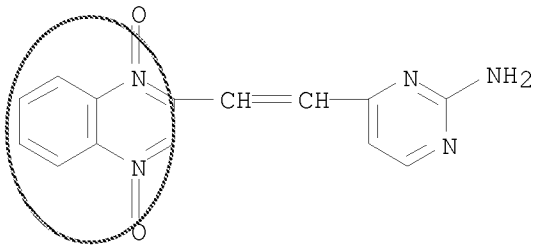
L8 ANSWER 76 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1978:484653 CAPLUS
DN 89:84653
OREF 89:12865a,12868a
TI Selective inhibition of cholera vibrio growth by 2-amino-4[(2-quinoxalinyl-N,N'-dioxide)vinyl]pyrimidine (CO1)
AU Bertolini, A.; Castelli, M.; Genedani, S.; Garzia, A.; Ferrari, W.
CS Inst. Pharmacol., Univ. Modena, Modena, Italy
SO Drugs under Experimental and Clinical Research (1977), 3(1), 201-9
CODEN: DECRDP; ISSN: 0378-6501
DT Journal
LA English
AB CO 1 (I) [59985-27-2] minimal inhibitory concns. (MIC) against Vibrio were 10-30 μg/mL, against Bacillus subtilis 30-125 μg/mL, and against B. anthracis 8-16 μg/mL. None of the other microorganisms tested were inhibited by ≤300 μg/mL. I, administered orally to mice at 500 mg/kg/day for 6 days, had no effect on intestinal microflora. I was lethal when given i.p. to mice, rats, and rabbits at 500 mg/kg, but was only slightly toxic when administered orally at 2000 or 4000 mg/kg.
IT 59985-27-2
RL: BIOL (Biological study)
(Vibrio comma inhibition by)
RN 59985-27-2 CAPLUS
CN 2-Pyrimidinamine, 4-[2-(1,4-dioxido-2-quinoxalinyl)ethenyl]- (CA INDEX NAME)



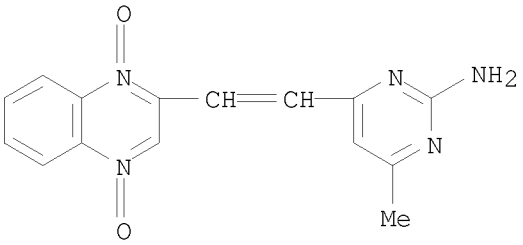
L8 ANSWER 77 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1978:83717 CAPLUS
DN 88:83717
OREF 88:13109a,13112a
TI Pharmaceutical composition for treatment of swine dysentery
IN Williams, Robert Dee; Garzia, Aldo
PA Istituto Chemioterapico Italiano S.p.A., Italy
SO Ger. Offen., 23 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2713906	A1	19771020	DE 1977-2713906	19770329
	US 4086345	A	19780425	US 1977-772863	19770228
	ZA 7701468	A	19780222	ZA 1977-1468	19770310
	BE 852982	A1	19770929	BE 1977-176200	19770329
	JP 52128235	A	19771027	JP 1977-34797	19770330
	FR 2346351	A1	19771028	FR 1977-9538	19770330
	FR 2346351	B1	19811127		
	GB 1542549	A	19790321	GB 1977-13444	19770330
	NL 7703551	A	19771004	NL 1977-3551	19770331
	ES 457383	A1	19780601	ES 1977-457383	19770331
	AU 7723813	A	19781012	AU 1977-23813	19770331
	AU 511916	B2	19800911		
	CA 1092027	A1	19801223	CA 1977-280721	19770616
PRAI	US 1976-672089	A	19760331		
	US 1977-772863	A	19770228		
	US 1976-672123	A	19760331		
	US 1977-771118	A	19770223		

OS MARPAT 88:83717
AB Substituted quinoxaline dioxides I (R = H or alkyl) are effective for prophylaxis or treatment of swine dysentery. For example, 2-[2-(2-amino-4-pyrimidinyl)ethenyl]quinoxaline 1,4-dioxide (I, R = H) [59985-27-2] was bactericidal to Treponema hyodysenteriae at <1 μg/mL and inhibited the growth of Vibrio cholerae at 10-100 μg/mL in vitro. I (400 g/ton in the feed) was curative to pigs with dysentery. I was prepared by reaction of 2.36 g quinoxaline-2-carboxaldehyde di-Me acetal di-N-oxide [32065-66-0] with 1.09 g 2-amino-4-methylpyrimidine [108-52-1] in 15 mL 99% HCO2H with catalysis by 1.15 g 96% H2SO4 at 45-50° for 10 h.
IT 59985-27-2P 65268-96-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, for swine dysentery treatment)
RN 59985-27-2 CAPLUS
CN 2-Pyrimidinamine, 4-[2-(1,4-dioxido-2-quinoxalinyl)ethenyl]- (CA INDEX NAME)



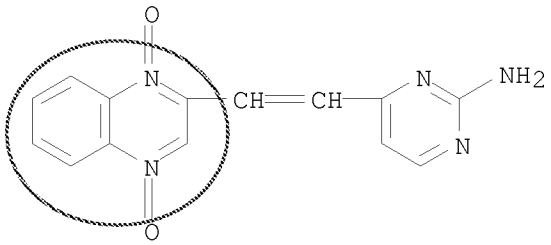
RN 65268-96-4 CAPLUS
CN 2-Pyrimidinamine, 4-[2-(1,4-dioxido-2-quinoxalinyl)ethenyl]-6-methyl- (CA INDEX NAME)



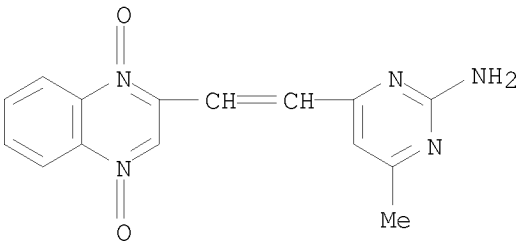
L8 ANSWER 78 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1978:50925 CAPLUS
DN 88:50925
OREF 88:8041a,8044a
TI Pyrimidinylvinylquinoxalines for combatting cholera
IN Garzia, Aldo; Ferrari, William; Bottazzi, Andrea
PA Istituto Chemioterapico Italiano S.p.A., Italy
SO Ger. Offen., 28 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2714157	A1	19771027	DE 1977-2714157	19770330
	US 4076815	A	19780228	US 1977-771118	19770223
	IN 144232	A1	19780408	IN 1977-CA394	19770317
	GB 1536393	A	19781220	GB 1977-11688	19770318
	BE 852913	A1	19770926	BE 1977-176150	19770325
	ZA 7701882	A	19780222	ZA 1977-1882	19770329
	CA 1069899	A1	19800115	CA 1977-275024	19770329
	DK 7701403	A	19771001	DK 1977-1403	19770330
	DK 143701	B	19810928		
	DK 143701	C	19820405		
	NL 7703465	A	19771004	NL 1977-3465	19770330
	FR 2346351	A1	19771028	FR 1977-9538	19770330
	FR 2346351	B1	19811127		
	ES 457359	A1	19780616	ES 1977-457359	19770330
	JP 52139087	A	19771119	JP 1977-37421	19770331
	JP 54037154	B	19791113		
PRAI	US 1976-672123	A	19760331		
	US 1977-771118	A	19770223		
	US 1976-672089	A	19760331		
	US 1977-772863	A	19770228		

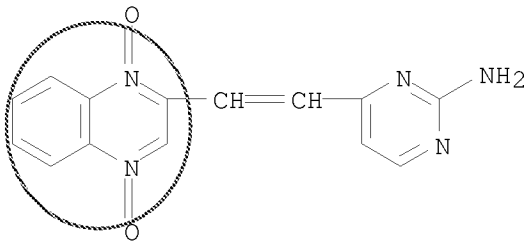
AB The quinoxaline derivs. I (R = H, Me) were prepared by the condensation of 2-formylquinoxaline N,N'-dioxide with II in the presence of an acid, e.g., H2SO4. I are useful for the inhibition of Vibrio cholerae microorganisms in waste water, as well as for the prophylactic treatment of cholera.
IT 59985-27-2P 65268-96-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, and cholera control by)
RN 59985-27-2 CAPLUS
CN 2-Pyrimidinamine, 4-[2-(1,4-dioxido-2-quinoxalinyl)ethenyl]- (CA INDEX NAME)



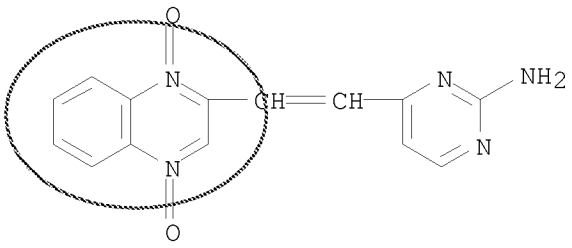
RN 65268-96-4 CAPLUS
CN 2-Pyrimidinamine, 4-[2-(1,4-dioxido-2-quinoxalinyl)ethenyl]-6-methyl- (CA INDEX NAME)



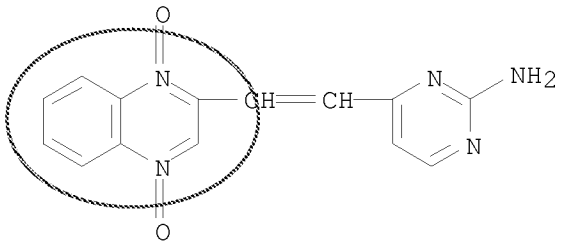
L8 ANSWER 79 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1976:487896 CAPLUS
DN 85:87896
OREF 85:14067a,14070a
TI In vitro induction of resistance to CO1 (2-amino-4-[(2-quinoxalinyl-N,N'-dioxide)vinyl]pyrimidine) in Vibrio cholerae
AU Bertolini, A.; Castelli, M.; Genedani, S.
CS Ist. Farmacol., Univ. Modena, Modena, Italy
SO Rivista di Farmacologia e Terapia (1976), 7(1), 113-18
CODEN: RVFTBB; ISSN: 0302-1750
DT Journal
LA Italian
AB Vibrio cholerae (V. comma), growing in media containing subinhibitor concns. of CO1 (2-amino-4-[(2-quinoxalinyl-N,N'-dioxide)vinyl]pyrimidine)(I) [59985-27-2] rapidly acquired strong resistance to the growth-inhibiting effect of this drug. However, the I-resistant strain retained its original sensitivity to 6-demethylchlortetracycline [127-33-3].
IT 59985-27-2
RL: PRP (Properties)
(Vibrio comma resistance to, induction of)
RN 59985-27-2 CAPLUS
CN 2-Pyrimidinamine, 4-[2-(1,4-dioxido-2-quinoxalinyl)ethenyl]- (CA INDEX NAME)



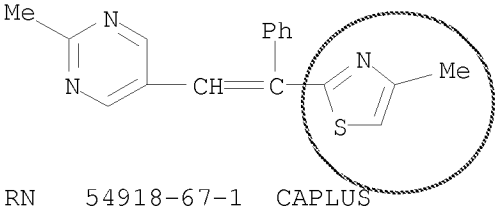
L8 ANSWER 80 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1976:487895 CAPLUS
DN 85:87895
OREF 85:14067a,14070a
TI Selective in vitro inhibition of Vibrio cholerae by 2-amino-4-[(2-quinoxalinyl-N,N'-dioxide)-vinyl]-pyrimidine (CO1)
AU Bertolini, A.; Castelli, M.; Genedani, S.; Ferrari, W.
CS Ist. Farmacol., Univ. Modena, Modena, Italy
SO Rivista di Farmacologia e Terapia (1976), 7(1), 107-12
CODEN: RVFTBB; ISSN: 0302-1750
DT Journal
LA Italian
AB 2-Amino-4-[(2-quinoxalinyl-N,N'-dioxide)vinyl]pyrimidine (CO1)(I) [59985-27-2] selectively inhibits the in vitro growth of Bacillus subtilis, B. anthracis, and Vibrio comma (V. cholerae). Its inhibitory influence on the growth of V. comma is not affected either by the contemporaneous growth of Staphylococcus aureus plus Streptococcus faecalis or by sewage. On the other hand, I does not grossly inhibit the growth of sewage microorganisms or significantly alter the colonic microflora in mice. Since I administered orally shows a very high LD50 in some common laboratory animals, this drug may be useful for the control of cholera.
IT 59985-27-2
RL: PRP (Properties)
(Vibrio, sensitivity to)
RN 59985-27-2 CAPLUS
CN 2-Pyrimidinamine, 4-[2-(1,4-dioxido-2-quinoxalinyl)ethenyl]- (CA INDEX NAME)



L8 ANSWER 81 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1976:487241 CAPLUS
DN 85:87241
OREF 85:13919a,13922a
TI Acute and subacute oral toxicity of a new antivibrio drug, 2-amino-4-[(2-quinoxalinyl-N,N'-dioxide)vinyl]pyrimidine (C01)
AU Castelli, M.; Genedani, S.
CS Ist. Farmacol., Univ. Modena, Modena, Italy
SO Rivista di Farmacologia e Terapia (1976), 7(1), 117-20
CODEN: RVFTBB; ISSN: 0302-1750
DT Journal
LA Italian
AB CO1 [2-amino-4-((2-quinoxalinyl-N,N'dioxide)vinyl)pyrimidine](I) [59985-27-2], which selectively inhibited the in vitro growth of Vibrio cholerae, showed a very low acute and subacute toxicity if administered orally to mice, rats and rabbits. In guinea pigs the oral LD50 was between 1 and 2 g/kg. Since acute toxicity in rats and mice was greater after i.p. than after oral administration, it was suspected that I was not readily absorbed by the intestinal tract. In view of the intensity and selectivity of the inhibition of V. cholerae growth, the absence of any interference by sewage on this antibacterial activity, the slight changes observed in the intestine microflora of mice receiving 500 mg/kg/day of the substance orally for 135 days, the quantities of the drug which can be administered by the intragastric route to rodents without signs of toxicity and the ability of Carassius auratus, Meiurus nebulosus and tadpoles to tolerate I concns. in the water of ≤ 0.5 mg/ml, it has been suggested that I might be useful for cholera treatment and for disinfecting an environment contaminated by V. cholerae without upsetting the biol. balance.
IT 59985-27-2
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study) (toxicity of)
RN 59985-27-2 CAPLUS
CN 2-Pyrimidinamine, 4-[2-(1,4-dioxido-2-quinoxalinyl)ethenyl]- (CA INDEX NAME)

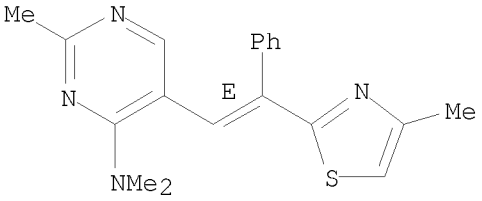


L8 ANSWER 82 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1975:97987 CAPLUS
DN 82:97987
OREF 82:15649a,15652a
TI Pyrimidine derivatives and related compounds. LXXXVII. Reaction of thiamine analog with diethyl benzoylphosphonate
AU Takamizawa, Akira; Harada, Hiroshi
CS Shionogi Res. Lab., Shionogi and Co., Ltd., Osaka, Japan
SO Chemical & Pharmaceutical Bulletin (1974), 22(12), 2818-23
CODEN: CPBTAL; ISSN: 0009-2363
DT Journal
LA English
AB Thiamine analogs lacking the 5-hydroxyethyl group (I, R = H, NH2, NHMe, NMe2, OMe) were treated with (EtO)2P(O)COPh. Comparison of reactivity in 4'-substituted thiamine analogs and those lacking the hydroxyethyl group suggests an interaction in the thiamine mol. between the pyrimidine ring and the hydroxyethyl group in an aprotic solvent. Reactivity at the 2 position (the active center in enzymatic decarboxylation) in 4'-substituted thiamine analogs may be affected by this interaction.
IT 54918-66-0P 54918-67-1P 54918-68-2P
RL: PREP (Preparation)
(from reaction of thiamine analog with diethyl benzoylphosphonate)
RN 54918-66-0 CAPLUS
CN Pyrimidine, 2-methyl-5-[2-(4-methyl-2-thiazolyl)-2-phenylethenyl]- (CA INDEX NAME)



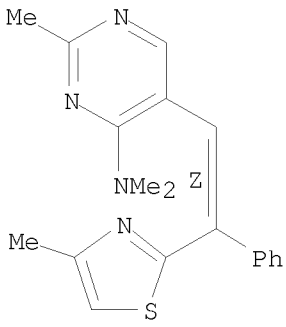
RN 54918-67-1 CAPLUS
CN 4-Pyrimidinamine, N,N,2-trimethyl-5-[2-(4-methyl-2-thiazolyl)-2-phenylethenyl]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

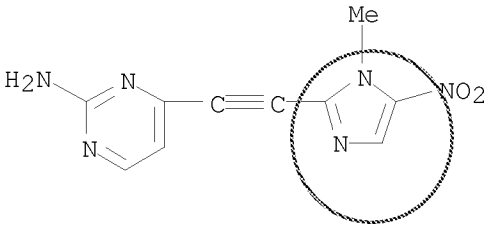


RN 54918-68-2 CAPLUS
CN 4-Pyrimidinamine, N,N,2-trimethyl-5-[2-(4-methyl-2-thiazolyl)-2-phenylethenyl]-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.


Me
N
N
NMe2
Z
N
Me
Ph
S

L8 ANSWER 83 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1975:661 CAPLUS
DN 82:661
OREF 82:127a,130a
TI In vitro antibacterial activity of 2-amino-4-(2-ethynyl-1-methyl-5-nitroimidazole)-pyrimidine, and metronidazole derivative with antitrimonad activity
AU Bertolini, A.; Castelli, M.; Poggioli, R.
CS Ist. Farmacol., Modena, Italy
SO Experientia (1974), 30(7), 757-8
CODEN: EXPEAM; ISSN: 0014-4754
DT Journal
LA English
AB The title compound (I) [53347-38-9], in addition to its trichomonocidal activity, was inhibitory to a number of bacteria. The antibacterial activity of the antitrichomonad drug has practical importance, since lesions induced by Trichomonas generally contain many undesirable bacteria. Although the commonly used drug metronidazole has broad systemic antiprotozoal activity, it has little or no chemotherapeutic effect on bacteria.
IT 53347-38-9
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(bactericidal activities of)
RN 53347-38-9 CAPLUS
CN 2-Pyrimidinamine, 4-[(1-methyl-5-nitro-1H-imidazol-2-yl)ethynyl]- (9CI) (CA INDEX NAME)



L8 ANSWER 84 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1974:491563 CAPLUS
DN 81:91563
OREF 81:14517a,14520a
TI Antibacterial 2-amino-4-[2-(1-methyl-5-nitro-2-imidazolyl)vinyl]pyrimidine
IN Garzia, Aldo
PA Istituto Chemioterapico Italiano S.p.A.
SO Ger. Offen., 31 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2358483	A1	19740627	DE 1973-2358483	19731123
	DE 2358483	B2	19800228		
	DE 2358483	C3	19801016		
	US 3882105	A	19750506	US 1973-364025	19730525
	ZA 7308720	A	19740925	ZA 1973-8720	19731114
	NO 135420	B	19761227	NO 1973-4420	19731119
	SE 402108	C	19780928	SE 1973-15633	19731119
	FI 57947	B	19800731	FI 1973-3570	19731120
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	BE 807617	A1	19740315	BE 1973-138008	19731121
	CH 590268	A5	19770729	CH 1973-16355	19731121
	FR 2207716	A1	19740621	FR 1973-41642	19731122
	NL 7316046	A	19740528	NL 1973-16046	19731123
	GB 1419806	A	19751231	GB 1973-54619	19731123
	ES 420768	A1	19760401	ES 1973-420768	19731123
	CA 998048	A1	19761005	CA 1973-186529	19731123
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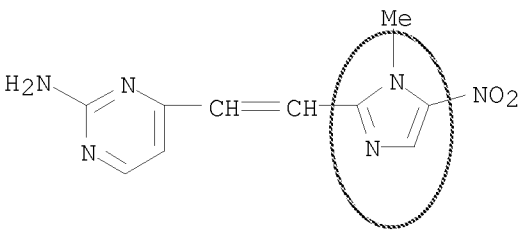
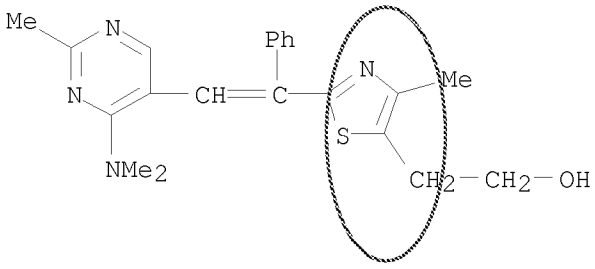
	JP 51045598	B	19761204		
	US 3969520	A	19760713	US 1974-521383	19741106
PRAI	US 1972-309483	A	19721124		
	US 1973-364025	A	19730525		

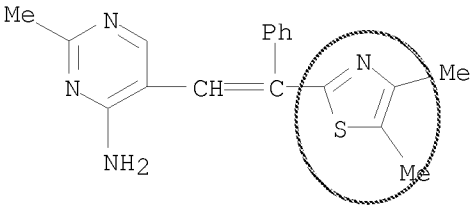
AB The pyrimidine I was prepared by heating 2-amino-4-methylpyrimidine and 2-formyl-1-methyl-5-nitroimidazole in AcOH for 4 hr at 55°. I was used as bactericide, protozoacide, and fungicide against various test organisms, especially against Trichomonas vaginalis in-festations of women.
IT 53409-75-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and bactericidal activity of)
RN 53409-75-9 CAPLUS
CN 2-Pyrimidinamine, 4-[2-(1-methyl-5-nitro-1H-imidazol-2-yl)ethenyl]- (CA INDEX NAME)



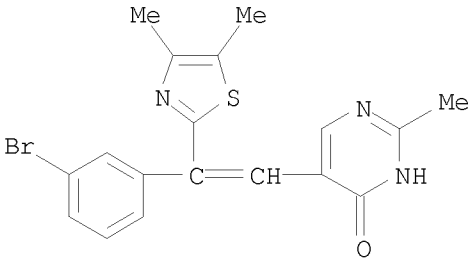
L8 ANSWER 85 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1973:466287 CAPLUS
DN 79:66287
OREF 79:10715a,10718a
TI Pyrimidine derivatives and related compounds. LXXVII. Reaction of thiamine analogs with diethyl benzoylphosphonate
AU Takamizawa, Akira; Harada, Hiroshi
CS Shionogi Res. Lab., Shionogi and Co., Ltd., Osaka, Japan
SO Chemical & Pharmaceutical Bulletin (1973), 21(4), 770-84
CODEN: CPBTAL; ISSN: 0009-2363
DT Journal
LA English
AB Reaction of thiamine analogs, 3-(arylmethyl)-5-(2-hydroxyethyl)-4-methylthiazolium derivs., with C6H5COP(O) (OEt)2 was carried out and an interesting difference in reactivity in aprotic solvent according to substituents and nuclei was observed
IT 42784-82-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 42784-82-7 CAPLUS
CN 5-Thiazoleethanol, 2-[2-[4-(dimethylamino)-2-methyl-5-pyrimidinyl]-1-phenylethenyl]-4-methyl- (CA INDEX NAME)



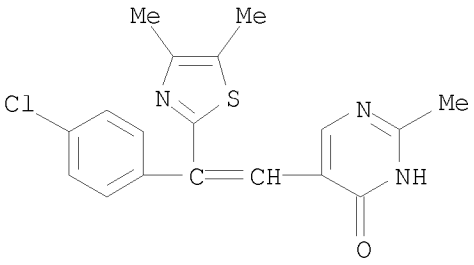
L8 ANSWER 86 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1970:435314 CAPLUS
DN 73:35314
OREF 73:5853a,5856a
TI Vitamin B1 and related compounds. CX. Rearrangements of α-hydroxybenzylthiamin and its homologs
AU Oka, Yoshikazu; Kishimoto, Shoji; Hirano, Hiroshi
CS Chem. Res. Lab., Takeda Chem. Ind., Ltd., Osaka, Japan
SO Chemical & Pharmaceutical Bulletin (1970), 18(3), 534-41
CODEN: CPBTAL; ISSN: 0009-2363
DT Journal
LA English
AB The structure of a product which is obtained by the reaction of thiamine with benzaldehyde was established as 2-[α-(4-amino-2-methyl-5-pyrimidinylmethyl)-α-hydroxybenzyl]-5-(2-hydroxyethyl)-4-methylthiazole (I). The mechanism of the reaction is discussed and the syntheses of several homologs of I as well as their chemical reactions are described.
IT 27350-87-4P 27350-89-6P 27350-90-9P
27375-19-5P 27507-34-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 27350-87-4 CAPLUS
CN Pyrimidine, 4-amino-5-[β-(4,5-dimethyl-2-thiazolyl)styryl]-2-methyl- (8CI) (CA INDEX NAME)



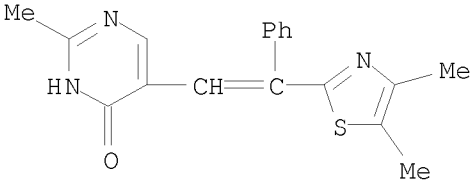
RN 27350-89-6 CAPLUS
CN 4-Pyrimidinol, 5-[p-bromo-β-(4,5-dimethyl-2-thiazolyl)styryl]-2-methyl- (8CI) (CA INDEX NAME)



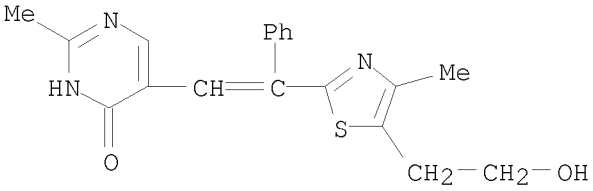
RN 27350-90-9 CAPLUS
CN 4-Pyrimidinol, 5-[p-chloro-β-(4,5-dimethyl-2-thiazolyl)styryl]-2-methyl- (8CI) (CA INDEX NAME)



RN 27375-19-5 CAPLUS
CN 4-Pyrimidinol, 5-[β-(4,5-dimethyl-2-thiazolyl)styryl]-2-methyl- (8CI) (CA INDEX NAME)



RN 27507-34-2 CAPLUS
CN 5-Thiazoleethanol, 2-[2-(4-hydroxy-2-methyl-5-pyrimidinyl)-1-phenylvinyl]-4-methyl- (8CI) (CA INDEX NAME)



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FULL ESTIMATED COST                                   470.14     655.15

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                      ENTRY    SESSION
CA SUBSCRIBER PRICE                                   -68.80     -68.80

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